THE USE OF MICROCOMPUTERS

IN CHEMICAL EDUCATION

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Two Teaching Package Disks to accompany Thesis. in back pocket.

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ABSTRACT

The use of computers for teaching in Chemistry has attracted widespread interest since computers became relatively common. However, despite considerable effort, no clear direction for their use as teaching tools has emerged. The advent of the microcomputer has recently brought the computer within the reach of all Chemists, and has resulted in a corresponding increase in the amount of software offered as teaching material. However, the apparent lack of direction available for new authors of software threatens both the credibility and effectiveness of the microcomputer in teaching. There was therefore a need firstly to investigate and secondly to evaluate techniques and strategies for the use of microcomputers in Chemistry.

To perform such an investigation, a stand-alone teaching package based on a microcomputer was constructed, with NMR chosen as its subject. The first part of the package was the inclusion of programs to present the background theory of NMR. Allowing students the opportunity to experiment and practise with newly-learnt skills was the next stage of the development. Exercises allowed students to analyse and to generate ^{1}H NMR spectra. Further exercises were needed to engage students in limited dialogue to further develop understanding. Analysis of the needs for the inclusion of such exercises indicated that an Author language would be useful. After consideration of the available software, a limited Author language was written.

A variety of exercises were included in the package using this language.

Evaluation of the package indicated that those students willing to use it did indeed derive considerable benefit from it. Analysis of student attitudes towards the package supported the view that it was successful. These attitudes also revealed a large potential for the use of similar packages in Chemistry.

An effective package was created, with its elements using a variety of styles of presentation to students. The strengths and advantages of each style were noted in the construction of the package, and are embodied in the teaching package. A number of useful software tools were also created. Important guidelines for the formal inclusion of CAL as a style of teaching in Chemistry were developed.

CHAPTER I

INTRODUCTION

Chemistry covers a vast and ever-increasing amount of material. This size has in turn necessitated the use of a number of tools for the teaching of Chemistry. One of these tools is the computer. A relatively recent innovation, the microcomputer, has had a profound effect upon computing and is similarly having an impact upon the use of computers for teaching Chemistry. However, although computers have been used for teaching for some time, their use has not always been effective. In addition lessons learnt from the use of larger computers are not necessarily applicable to the new type of machine.

The intention of this thesis, therefore, was to investigate and to evaluate the various techniques and strategies for using microcomputers in the teaching of Chemistry. The investigation concentrated upon the use of the microcomputer as a self-contained exercise in a structured part of the educational system, since it was considered important that the microcomputer be used for teaching in a direct manner, rather than a peripheral one, as just another sophisticated teaching aid.

1. A BRIEF HISTORY OF COMPUTER ASSISTED LEARNING

A survey of the literature on computers in education will reveal the large number of phrases and accompanying

acronyms that have been used to describe this activity. Computer Assisted Learning, CAL, is the phrase used throughout this thesis to describe the general area under study, although Computer Aided Instruction, CAI, is also widely used in the literature, at times interchangeably with CAL.

The development of Computer Assisted Learning can be traced back to the Programmed Instruction (PI) movement of the early 1960s. B.F. Skinner, an experimental psychologist, revived and extended the ideas of S.L. Pressey, leading to the use of machines to deliver and mark material according to a set programme (Skinner, 1958).

Pressey's ideas centred on using mechanical aids to do "many things now done in our schools and colleges in very unnecessarily laboured and enthusiasm-killing fashion" (Cronbach, 1963, p.410). He thought that such aids "would leave the teacher more free for ... the important work" through the relief of some of the mechanical tasks of the profession. Skinner's work was based on his theory of learning, which held that, when asked a question, the student "retains the responses that are confirmed" rather than learning from mistakes. To ensure that students would be likely to answer most questions on a piece of work correctly, Skinner devised the technique of presenting the necessary information and increasing the difficulty of questions "in small steps". Unlike Pressey, who envisaged a miscellaneous collection of exercises, Skinner's method involved careful attention to the presentation. The essence of this method, Programmed Instruction (PI), is therefore

the programming. PI basically involved presenting information and asking the student questions of gradually increasing difficulty. Progression to the next question depended on a correct response. There were two methods of dealing with incorrect answers. In linear PI the question was simply repeated, while in the more complicated branched method help was given to the student, often in the form of hints, and questions of equivalent difficulty were posed before moving on.

Mastery of a single section of material was said to be achieved upon attainment of a high proportion (80% was common) of correct first answers. Students demonstrating such mastery proceeded to more difficult work, while further equivalent series of questions were available for the others.

The computer, with its processing and decision-making abilities seemed to be the ideal medium for the implementation of this strategy, with the aid of a tutorial style of program. Unfortunately, when presenting quantities of simply textual material, there is the possibility of reducing the computer to the role of "page turning".

There was considerable further thought given to the use of computers in education in the mid- and late-1960's, but, as outlined by Nievergelt (1980), no clear directions emerged. It was evident that the basic hardware available was inadequate, as interaction with the computer was limited to cumbersome teletypes with a small range of available characters (upper case letters and numbers) and slow, often noisy output. A more flexible and convenient delivery

system was required, but the cost of visual display units (VDU) was still too high and their performance inadequate. It was also suggested that the use of computers in teaching needed to be more thoroughly understood before further material was produced. The obvious reply made to both of these suggestions was "... if you are going to wait ... I am afraid we will never get the first system up. Somewhere along the line we have to be willing to ... get some experience" (Atkinson, 1967).

The simplest form of CAL, a style often known as "drill and practice", was probably the most obvious with which to begin at this stage, being relatively easy to implement and use on the available hardware. It was, as a result, rather over-emphasised as evidenced by the tendency of researchers in the United Kingdom to equate Computer Aided Instruction (CAI), the equivalent of CAL in the United States, with drill and practice (Moore and Thomas, 1981). An outline of drill and practice appears in a later section.

There was still considerable optimism expressed by serious researchers, even though progress was apparently slow. For example, the prediction was made that individualised drill and practice programs would be in widespread use in schools by 1978, with the more advanced "tutorial" style programs to follow shortly after, even though the author admitted that "as yet we have little operational experience in precisely how this should best be done" (Suppes, 1968). Even comments such as "most of the problems ... have yet to be solved" (Silberman, 1968) did not deter some enthusiasts from making extravagant claims

about the future use and effectiveness of computers in education.

By the early 1970s general enthusiasm had lessened somewhat. Certainly many educators had become more sceptical about the effectiveness of CAL as a teaching tool. The general trend amongst CAL researchers was away from tutorials and drill and practice sessions with major emphasis being placed on simulations. One of the guidelines for preparing software for the large Plato project at the University of Illinois was that "The computer should be used as much as possible to simulate results in models ... rather than simply turn pages" (Bitzer and Skaperdas, 1970).

Programming has been advocated as the best way to use a computer to teach (de Laurentiis, 1980). Proponents of Learning by Interactive Programming (LIP) suggested that the best use of a computer would be made when students are directly involved with it at a basic level. Papert (1980) wrote that "... the computer is being used to program the child. In my vision, the child programs the computer."

The LIP movement became more widespread, possibly as a reaction to previous misuses of Computers in education. It was pointed out that there is little value in "putting a tutor into the computer to intervene between the student and the subject matter" when it is not necessary. "The major objective ... is to put the student in contact with the subject matter so that he can work with it directly" (Glaser, 1970).

One enduring example of LIP is the Logo System (Papert, 1980). In the modern versions of Logo the user

controls a small animated "turtle" which can be moved around a graphics screen (the term "turtle" arose from the original mechanical device), using a variety of simple commands such as MOVE or TURN. It is said to have a "magic" pen attached to it which can be lowered onto the screen (PENDOWN) and will draw lines in various "colours" wherever the turtle goes. Students combine groups of instructions into procedures, which can in turn be used to accomplish tasks of increasing complexity. The authors of Logo are enthusiastic about it and LIP in general (Papert, 1980) and in support of this Logo has gained some acceptance in schools. The graphics package itself has attracted some attention and even appears as a standard addition known as "Turtlegraphics" in the teaching package used for this project.

Predictions, made in the early 1970s, about the future of computers in teaching using the older styles of CAL were still confident, although more guarded than in the past. An example of this is a comment made in 1970: "more highly-enriched tutorial CAL will spread more slowly as the effort needed to develop it properly and the cost of production increase. By the mid 1970s it should be commonplace ..." (Holtzman, 1970).

Much was written on CAL throughout the decade, varying from the general, such as the importance of graphics, to the specific ("How to achieve an effective screen layout") and from the fundamental to the trivial. Overall there was much repetition and very few publications managed or even attempted to provide a detailed guide for writing CAL

software for the inexperienced author, difficult as producing such a guide might be. There have been some very useful papers appearing recently, which describe many of the requirements for producing good CAL material (e.g. Nievergelt, 1980), but the inexperienced CAL author would still be bewildered by the range of options available. Developments in technology and in particular in low-cost computing towards the end of the decade ensured that there would be a large number of these inexperienced authors.

There were many successful projects producing good software throughout the 1970s. The most relevant of these to CAL in the Chemistry Department at Canterbury University was the CALCHEM project (Ayscough, 1977), with experiences with some of the programs provided by CALCHEM having profound influences upon the direction of this project. As more research groups became established however more "what we have done" papers appeared, some with useful offers of software (Moore, 1979), but others of less value (Gull, 1980). This trend has accelerated with the advent of the microcomputer.

2. TYPES OF CAL

Often specific CAL programs are assigned to one of several categories depending on outward form. While the various labels are useful the distinctions are often of degree rather than type. Classifications (for example, Dence, 1980) commonly identify the five general types of CAL: drill and practice, tutorial, dialogue, simulation and programming.

1) Drill and Practice

Drill and practice programs are the simplest in form and are aimed at reviewing and reinforcing material which is already known by the student user. Generally a question is put to the student and a response evaluated. If judged correct the answer is confirmed and the next question given. How incorrect or partially correct responses are dealt with depends upon the sophistication of the approach in the program. Extremes of this approach may vary from simple rejection and repetition of the question, to the provision of useful hints, with records kept by the computer in order to pose similar questions later in the session.

While the drill and practice programs are probably the easiest to implement and hence the most widely available, they are also the easiest to misuse, for example by attempting to use them to teach completely new material. Reactions to poor use of drill and practice programs are often extremely negative.

2) Tutorial

Tutorial programs present information to the student directly, with progression in difficulty. Interaction between student and computer serves to set the pace of the process and may also be used to assess student progress and difficulties in understanding the material. Provision can therefore be made for short-cuts for the more able student and extra detail for the slower student. The tutorial style of Computer Assisted Learning was probably the earliest

approach, with many features in common with the Programmed Instruction method of teaching.

3) Dialogue

In a completely free dialogue situation the student would control the major direction of the presentation, with the computer taking the part of a knowledgeable tutor. This style is often termed Socratic because the student is encouraged to investigate and extend his knowledge as in a discussion, rather than in a lecture. Obviously such a dialogue would require a sophisticated computer system to support it and it is not a style of CAL widely used at present with microcomputers. Many tutorial style programs do however incorporate more limited dialogue features capable of implementation on microcomputers.

4) Simulation

Computers are particularly suitable for simulating many processes, especially those which can be expressed in terms of a mathematical model. Simulations may be used, for example, to observe the effects of altering parameters in dynamic processes especially those which are difficult or dangerous to perform as a "live" experiment or for which the time scale is inconveniently short or long. A good example is a game designed to study the Contact Process (production of sulphuric acid) for school chemistry classes. Manipulation of key variables such as temperature, pressure and concentration of reactants in the rate determining step in order to achieve the lowest cost of product has proved to be both useful and popular with students.

Simulations are of value mainly to provide experience and appreciation of the entirety of a process, rather than as a direct teaching tool. They should therefore be used in situations where the user has some background knowledge. Simulations are no substitute for the practical experience that may be gained from "live" experiments.

5) Programming

As has been noted, programming has been advocated as the best way to use a computer to teach (de Laurentiis, 1980). Proponents of Learning by Interactive Programming (LIP) suggest that the best use of a computer is made when students are directly involved with it at a basic level. LIP is said to encourage students to develop understanding of complex processes by the design and construction of simple, self-contained procedures and by combining these in the construction of a model for the process.

3. MICROCOMPUTERS

With the relatively sudden arrival and rapid proliferation of the microcomputer the possibility was raised of overcoming some of the problems associated with CAL based on large computer systems. Being self-contained and possessing the capacity for fast graphics operations on a VDU were obvious advantages, along with the relatively low cost. Early doubts about the capacity of the microcomputer continue to be eroded as the amount of computing power per dollar steadily increases.

Reactions to suggestions for the use of microcomputers for CAL have been mixed. Disappointments with the claims of earlier enthusiasts have left many educators sceptical, even though (or perhaps because) a new generation of supporters has emerged. Despite this scepticism the microcomputer is having a significant effect on CAL. The cost factor alone means that computers are within reach of the general public for the first time.

However there is a real possibility that the use of microcomputers for CAL could meet the same fate as Programmed Instruction within the educational establishment. A parallel between the two forms has been drawn by Ragsdale (1982), who noted that "the flood of PI material hastily prepared by inexperienced authors" more than cancelled "the sequence carefully prepared by experts". Many manufacturers of microcomputers actively promote the educational uses of their products and, whether intentionally or not, seem to imply that learning to program is equivalent to learning to produce good CAL material. Some of the early teaching material has left a good deal to be desired. Fortunately there are agencies aimed at evaluating and distributing good CAL material. Project SERAPHIM (Moore, 1980b), for example, has some significance for CAL Authors in Chemistry.

4. THE AIMS OF THE PROJECT

It has become increasingly apparent that there is a real need for clearly stated goals in CAL in Chemistry, if not in the entire field of Computer Assisted Learning. Despite the length of time that computers have been used in

education, a set of standard rules for their effective use has yet to be developed and authors must generally rely upon common sense and experience when developing CAL material. In addition there seems to be the real possibility of another, but perhaps more damaging, negative reaction to the use of computers in education being precipitated by a large volume of software which is poorly designed and lacking in depth. As has been noted, "there is extremely little good computer-based material available" (Bork, 1984).

There were therefore three general aims in the project.

1. To investigate the techniques for the effective use of microcomputers in Computer Assisted Learning in Chemistry and to establish guidelines.

2. To create a set of tools for the development of CAL systems.

3. In addition to the physical construction of a self-contained teaching package, to attempt to find the places in the current educational system for the best use of such CAL exercises, with particular interest being placed upon the student viewpoint.

Since many topic areas in Chemistry have teaching problems in common, it was felt that the development of CAL software designed for one area would be widely applicable to others. It was therefore decided to explore in depth the application of Computer Assisted Learning to one broad subject area in Chemistry.

5. CHOICE OF SUBJECT AREA

There were two important initial considerations in the choice of subject area. The first was that it was necessary to chose a topic which would suitably illustrate the main principles of Computer Assisted Learning. The second was the establishment of a CAL Teaching Package adaptable to a wide range of Chemistry topics. Clearly the criteria for such a selection included ensuring that the completed package would be useful, that it could easily be included in the established course structure and that the topic was of some importance in Chemistry.

The topic chosen was that of Nuclear Magnetic Resonance (NMR), to be presented principally at a second year undergraduate level. This choice was made for four major reasons:

1. NMR had no formal coverage at that student level,

2. NMR was included to some extent in the laboratory course where the computer exercise could be introduced with little disruption,

3. there would be immediate applicability to other spectroscopic techniques (Infrared, Ultraviolet), as well as to general Chemistry topics,

4. there were definite indications for the use of graphics, potentially the feature of greatest importance in using the microcomputer.

The importance of NMR in Chemistry is well established. "NMR is the single most important physical tool available" (Leyden and Cox, 1977, p.1) was a statement echoed by many Chemists and supported by the considerable

expansion of both facilities and scope of use of NMR, even during the period of this research. The technique is now widely available to undergraduate students for routine use in laboratory sessions.

The major applications of NMR have been in Organic Chemistry, especially for obtaining structural information of compounds and the identity of molecules, or parts of them. In addition data concerning intermolecular motion, internuclear distances, rate constants and energy barriers associated with rotations are some of the other useful benefits of this technique.

Accompanying the increase in interest in NMR has been an increased emphasis on educational coverage of the topic. NMR is now presented in some detail at the second year Chemistry level at Canterbury and a proton NMR spectrometer is available for undergraduate use in conjunction with the laboratory course.

(1) Preliminary Investigation

As has been indicated, the exercise was intended for use by second- and perhaps third-year undergraduates. Access to students was relatively easy and unobtrusive through the laboratory sessions and the number of students was large enough to give a reasonable sample size, but small enough to ensure that every student had access to the exercise. It was important at the outset to attempt to assess the specific needs of the students concerning NMR.

What experience second year students had with Nuclear Magnetic Resonance was through the laboratory classes, rather than through formal lectures. In the laboratory

emphasis was placed upon the use of NMR in conjunction with other spectral techniques, to deduce the identities of compounds. At the beginning of the third year course, students spent one laboratory session using a mainframe computer for CAL work, to review spectroscopic methods. Two CAL exercises, a tutorial exercise and a proton NMR spectrum analysis program for practice, proved to be useful in providing an indication of initial areas for investigation. Descriptions of these exercises appear in Ayscough, Morris and Wilson (1979), the tutorial as "S200" and the spectrum analysis as "S201".

A pattern emerged in the very first session and was repeated with each group of students. The tutorial lesson on NMR would pose a series of questions to the student. Upon failing to answer correctly at least six out of nine, the undergraduate was told that his level of understanding was not sufficient and that he should research the topic more thoroughly. The lesson was then terminated. With the aid of the printed output of that attempt (the terminal was a teletype device, producing text at 300 baud), which contained the answers to the questions, most students managed to reach a second set of questions upon attempting the lesson for a second time, by answering the required number of initial questions correctly. Unfortunately the level of difficulty of the second set was somewhat higher than desirable.

In many cases the entire lesson became little more than a conversation piece for the students and the demonstrator. Admittedly the students were recommencing

studies after a long summer vacation and, in typical fashion, denied any previous encounters with Nuclear Magnetic Resonance, but even so as a stand-alone device for aiding recall of material the program was not a success. That there was much useful material contained in it was not in doubt. The unfortunate fact was however that the information was not readily available.

A second program on NMR dealt with the analysis of proton spectra. While suffering from the problems associated with a mainframe, for example fluctuating response times, the lack of graphics and some deficiencies in structure, the program was an effective enough tool, provided some initial help was given to students. In fact the idea behind the exercise was an inspiration for a part of the final CAL teaching package (Chapter IV).

Watching and listening to students using the CAL programs indicated one feature necessary for a stand-alone package: the availability of background material. Students needed further explanations on many occasions and, in a supposedly self-contained package, these would have to be provided. If constructed correctly, a background program could act either as a patient tutor covering the whole topic, or as a source of quick-reference material. Formulation of such a background program was judged to be the best starting point for the construction of the teaching package.

(2) Defining the Subject Area

The material to be presented in the teaching package was collected from four main sources: textbooks, lectures,

laboratory exercises and the previously-noted CAL lessons, the latter being used to check the coverage of material against an outside reference.

There were five specific objectives which emerged from consideration of the above sources. Students should acquire: 1) a background knowledge of the qualitative theory of NMR, 2) an understanding of the basics of Chemical Shift as related to the electronic environment of the nucleus, 3) a feeling for the general trends and common values of Chemical Shift, 4) an understanding of the source of Spin-Spin Coupling and 5) the opportunity to practise with the analysis of spectra.

Assessment of the possible contents of the teaching package proved to be more of a matter of careful elimination than of construction. The inclusion of every aspect of NMR would clearly lead to student confusion. The extent of coverage then hinged upon finding an adequate abridgement of the topic that was internally consistent and yet sufficiently detailed to provide a basis for a complete treatment. The full details of the areas covered appear, with the derived methods of presenting them, in succeeding Chapters.

Chapter II

CONSIDERATIONS OF HARDWARE AND SOFTWARE

There was no choice in the selection of the microcomputer for use in the research, since there was only one type available in the Chemistry Department at the time. However, before commencing construction of the package, an assessment of some of the capabilities of the microcomputer was made. A particular component of this assessment was the comparison with the earlier machine used in the department for Computer Assisted Learning work.

A further consideration in the initial preparation for the package was the choice of a programming language. The merits of the various possible languages in the limited range then supported on the available microcomputer, were assessed and a choice made, although the use of languages was to come under further scrutiny later in the research.

1. CHOICE OF COMPUTER

The microcomputer used for this research was an APPLE II+, a general purpose stand-alone computer, expanded to sixty-four kilobytes of memory. Dual 5 1/4 inch floppy disk drives, each with 140 kilobytes of storage were attached. Three programming languages were supported: assembler (machine code), BASIC and **Pascal**. One of the most attractive characteristics of the machine was the availability of medium resolution graphics (192 by 280).

Most interaction with the computer occurred through a keyboard and a visual display unit. The output on to the VDU could be in either of two forms, as text (24 lines of 40 characters) or as graphics. Of some interest were two further interactive devices, the speaker and the "games paddles". The small speaker enabled sound to be produced under program control. The "games paddles" (joystick), were essentially variable resistors whose values were converted to numbers for internal use following user input.

(1) The previous CAL Machine

Prior to the commencement of this project, Computer Assisted Learning work within the Chemistry Department was conducted on the timesharing Burroughs B6700 computer, which serviced the entire University. This computer, with its remote teletype terminals, was not ideally suited to CAL work. The relatively low output speed, limitation to upper case characters on hardcopy devices, and variable response times often made the CAL sessions rather tedious. Computer-generated interactive graphics are rare on mainframe computers and so it was in this case. Diagrams were either crude approximations made from text or were "visicards", which were entirely external to the computer. In addition the cost of running lengthy sessions for interactive work was not insignificant.

The major advantage of a mainframe computer over a microcomputer is power. In terms of sheer computing power and storage ability a mainframe computer was obviously superior, although many modern microcomputers approach some older mainframes in capability. However while the features

of power and storage ability are desirable, their absence in a microcomputer is offset by the immediacy of response, low cost, physical transportability and graphics capability. The last feature is possibly the most important (Bork, 1975b).

(2) Advances in Technology

The microcomputer field has been characterised by rapid developments. Most of the major advances relevant to this project have been in the form of software improvements, although later generations of the APPLE computer possess improved hardware.

Three developments were particularly significant to this research. The first was an operating system update. This supported the ability to enter conveniently from the keyboard both upper and lower case characters, where previously lower case was only available in graphics mode and only after manipulating ASCII character codes. It also included the facility to initiate program execution from within another program. The second development was a number of improvements to the documentation of the APPLE operating system which, for example, led to an editor for graphics characters. The third was the means to compress the eight kilobytes of memory required for a graphics display into a minute fraction of that amount for disk storage (Green, 1983). This development was important in making the MASTER authoring language (Chapter VI), an important part of the final teaching package, into a viable proposition.

2. THE CHOICE OF PROGRAMMING LANGUAGE

Although three languages were supported by the APPLE computer at the time of commencement of the project, the choice of programming language was between only two: implementations of BASIC and UCSD **Pascal**, respectively known as APPLESOFT and PASCAL (Apple Reference Manuals). Assembly (machine) language programming was not considered suitable, since its only real advantage, speed, was considerably outweighed by the complexity of the language, the difficulty of comprehending program listings and the tedium involved in its use.

Apart from outward form, APPLESOFT and PASCAL differ in a more fundamental way. In the PASCAL system the source program is "compiled" before execution, while in APPLESOFT, the source program is "interpreted". Thus APPLESOFT programs are interpreted line by line, with each line being first converted to machine usable form and then executed. Each time a line is encountered it must be reinterpreted. In contrast a PASCAL program is "compiled", analysed for syntax and consistency, and another entity, a "code" file, is produced. This file can be considered to be in machine usable form and will therefore execute rapidly. However an alteration requires a PASCAL program to be recompiled, which can be a lengthy procedure. An APPLESOFT program can be executed immediately after making changes. Schuyler (1979) discusses these differences.

It seemed likely that the speed of execution factor would demand the choice of PASCAL, as the risk of losing student concentration through slow responses was too great

for APPLESOFT programs of any complexity. Comparison of some of the other features of the two languages confirmed this preference. The structured form of the **Pascal** language ensures greater readability of source programs and clearer overall design. Author definition of data structures for internal and interactive use is possible, with the compulsory definition of all internal variables being a useful aid for the minimisation of errors. The language itself is, in addition, more "standard" than APPLESOFT. That is, a program written in PASCAL is likely to require little change to be able to be compiled in a version of **Pascal** implemented on another computer.

One further consideration added strength to the choice of PASCAL as the most appropriate language to use initially in the teaching package. While both PASCAL and APPLESOFT had graphics capabilities, PASCAL had the significant advantage of TURTLEGRAPHICS, a "standardised" graphics package, which increases the possibility of transporting programs to other types of computer.

The choice of the PASCAL language was therefore made for its superior and more adaptable computing ability, its apparent transportability and its significantly improved documentation, although the time involved in making changes to a program was significantly greater than in APPLESOFT. As it transpired, the choice of a language for use in the teaching package, or indeed any Computer Assisted Learning work, proved to be of increasing interest throughout the research.

Chapter III

THE TUTORIAL PROGRAMS

The need to provide background material was deduced from the experiences of students using mainframe-based Computer Assisted Learning lessons (Chapter I). Since the aim of this research was to design a self-contained package, the first priority was considered to be the production of a tutorial-style program to present the relevant background information on NMR.

The number of approaches to presenting the basic theory of NMR is apparently almost equal to the number of text books on the subject. Since textbooks were to be the principal source of information the preparation of a detailed, sequential series of statements to put to students was a matter of eliminating material not considered essential. In addition possible distracting influences, such as the mention of quantum mechanics and Fourier transformations, were avoided where possible. Detail of the material presented appears later in this Chapter.

1. OUTLINE OF APPROACH AND DEVELOPMENT OF PROGRAMS

The final form of the tutorial part of the teaching package differed markedly from that initially envisaged. At first it was thought that the information, which had been prepared in a sequential fashion, would necessitate the production of a similarly sequentially developing program.

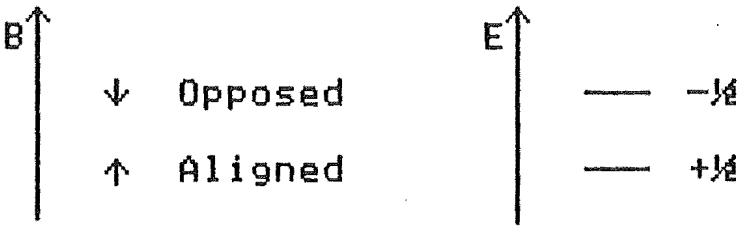
With this approach there was a possibility of adopting the wrong emphasis when producing a program. As was the case in the early stages of this project and as can been seen in many examples of CAL, it is easy to fall into the trap of allowing ease of programming rather than teaching considerations to determine how material is presented. The result is usually the style of programming known as "page turning", which is characterised by four steps: 1) Fill the screen with text, 2) pause, 3) clear the screen and 4) go to step 1.

This was the style used in the initial stages of the project, although it was enhanced with some of the features of the computer. Sound was used to underline important points and also to remind students that some action was required. For example the "end of page" message (Figure 3.1) had an accompanying tone. To help with the understanding and memory of the important equations, the game paddles (referred to as the joystick) were used to allow student interaction. Altering the setting of a paddle caused a flashing arrow, which was pointing at one of the terms in the equation, to move. Pressing a key resulted in some information, in the form of a brief comment, to be made on that term (Figure 3.2).

(1) The Effect of Feedback

When writing CAL programs for a particular subject it is important to seek regular assessment of the produced material by relatively objective experts in that subject.

Let's put our magnet in a magnetic field



There are two orientations possible, corresponding to the two values of m: (with I = ½ we have m = −½ and m = +½).

Hence we get two distinct energy levels.

>>>> Press <RETURN> to cont. <<<<

Figure 3.1

End of "Page" message in PART1

PAGE C

The energy of each level is given by :

$$E = -\frac{\gamma h}{2\pi} mB$$ <cont>

The selection rule for NMR is $\Delta m = \pm 1$, and hence the energy transitions are :

$$\Delta E = \frac{\gamma h}{2\pi} B$$ <cont>

and, as $\Delta E = h\nu$ ...

$$\nu = \frac{\gamma B}{2\pi}$$ <cont>

"γ" Gyromagnetic ratio (a constant)

Figure 3.2

Important equations in NMR

Such feedback helps to ensure that programming details do not diminish the quality of the final product. This type of review could be termed "Content Assessment".

A result of such an assessment was the decision to divide the material to be covered in the tutorial programs into two sections, in order to facilitate the introduction of an interactive section, which would allow students to review the material they had covered. The first program, PART1, was to contain the Introduction and Chemical Shift information, while the second, PART2, was to deal with Spin-Spin Coupling. The opinion was expressed that the concepts involved in this latter topic were difficult for students to grasp and the evaluation of student problems with NMR (completed at the commencement of this project) supported this. The spread of coverage of material in PART2 was consequently reduced and the overall layout was improved, with less text and more diagrams displayed.

(2) Style of Display in the Tutorial Programs

Student reception and response to programs is possibly the most important measure of their effectiveness and, as in the case of Content Assessment, all comments made are worthy of careful consideration. In this case a significant development arose from consideration of student responses.

The need to give students the opportunity to review previous information was highlighted by student comment in response to early testing of PART1. In order to provide the "review" capability the data to be presented had to be organised into a series of sequentially-developing, but essentially self-contained units, rather than as a series of

single statements. Upon request (by a single keystroke) the user could select any unit in the program for study, which not only allowed a review of previous information, but also allowed the program to be recommenced at any part following a break. The comparison between the program and the text book was fostered with the naming of each unit as a "page", with each having a unique label. Letters, instead of numbers, were used to identify each unit to ensure that only a single keystroke was necessary to identify a page.

The "paging" feature, first implemented in PART2, has proved to be invaluable as a part of the teaching package. When the two programs were compared by students in an early testing period, opinion overwhelmingly favoured PART2 over PART1, even though the latter had the advantages of completeness and an interactive section to help test student knowledge.

The improvement in approach initiated in PART2 was both fundamental and crucial to the production of CAL programs. It must be remembered that the information is always the key element and the method of display should reflect this. Presentation of text should therefore proceed in three general steps.

1. The screen is cleared, or at least changed significantly to signal a new section of material.

2. Information is to be presented in small amounts, with successive data resulting in screen modification, rather than complete renewal. Where possible previous key points remain on display. This step continues until a section of work is satisfactorily covered.

3. The first step is repeated, although this step is optional, with a teaching exercise being a continuous modification of a screen. It has been found however that having clear section delimiters (a definite end to a series of displays) allows students to pause and reflect on the work covered. For instance by clearing the screen at the end of a section of a "page" the modular aspect of the programs is emphasised.

Even when having to present information which must be sequentially developed, it is not only possible but very desirable to avoid mere "page turning". The tutorial exercises in this computer are best described as using the computer as an "electronic blackboard" (Nievergelt, 1980).

(3) Questions accompanying the Tutorial Programs

Each program concludes with a series of questions. Typically the tutorial style of program is presented as being short bursts of text interspersed with some form of interaction, usually in the form of short-answer or multichoice questions. However, it was felt that such a style would detract from the presentation by continually forcing the students to change stance from assimilation to what can often amount to regurgitation of information.

For two other reasons a short series of questions was included at the end of each program rather than throughout. As became apparent the process of using questions to encourage learning on the part of student users is not straightforward and should not be taken lightly. Having the questions separate from the main body of the program allowed separate development and was in keeping with the modularity

of the design. The second reason related to the basic philosophy of the package. Students more highly motivated to learn will learn more; an assertion bourne out in the testing of the package (Chapter VII). The teaching package was designed to allow learning to proceed at the user's pace rather than to aggressively demand that users learn everything immediately.

The purpose of including the questions was to review important points in each program by presenting the information from a different viewpoint to that previously displayed. In requiring student users to put some effort into thinking about the material it was hoped that it would therefore be remembered better. Students were allowed up to two attempts at each question and the correct answer was given in full in all cases. The style of presentation of the questions contrasted with the main program, with the adoption of a more personal tone; the more frequent use of the personal pronoun being the most obvious example. Students responded to this feature with surprising enthusiasm and, in general, indicated that each series of questions was useful. A score was kept for each student by the computer, to allow an assessment of their retention. This score appeared to be valuable, especially as students would often return to the main program in order to review problem areas as indicated by the questions.

It is interesting to note that students assumed that they would be tested in some way by the computer, and the questions seemed to fulfill this expectation.

2. THE FIRST TUTORIAL PROGRAM

PART1 was constructed with simplicity in mind, but even so needed some explanation and comment for its users. The first display was therefore an introduction which included the details of how to access the review/preview capability using the ESCape key. This key was used because of its position on the keyboard (it is relatively isolated in the top left hand corner) and also because it does not usually appear on a typewriter keyboard. When the key was pressed a list of available options was displayed, with each essentially being a short summary of the relevant "page". These summaries were:

A. Introduction to the program,

B. Nuclear Spin,

C. Equations of Energy States,

D. Transitions between States,

E. Introduction to Chemical Shift,

F. Formula and Derivation of Chemical Shift,

G. Factors influencing Chemical Shift,

H. Examples of Hybridisation Effects,

I. Examples of Electronegativity Effects,

J. Using the Joystick,

Q. Proceed to the Questions,

X. Exit the program and return to the menu.

The concept of Nuclear Spin was introduced on Page B with a series of statements supported by examples. The number of possible orientations for a nucleus of spin I was presented, but attention was immediately narrowed to the two nuclei, ^{1}H and ^{13}C (with I = 1/2), used throughout.

There was a conscious decision made to include both nuclei in the tutorial exercise in order to make use of the best features of each (for example ^{13}C proved to be less confusing for illustrating coupling) and to encourage familiarity with ^{13}C NMR spectra.

By choosing two nuclei which have two possible orientations in a magnetic field, it was thought that students would be quick to draw the parallel with electron spin. This was seen to be the case. The two energy levels resulting from the orientations are illustrated on Page B (Figure 3.1).

Page C ("Equations of Energy States") displays a series of equations as illustrated in Figure 3.2. As has been mentioned previously the student, using game paddles or a joystick, positioned a flashing arrow above a symbol and pressed a key to receive a short comment on the symbol. In Figure 3.2 the arrow points to the "γ", the symbol for the gyromagnetic ratio. To move on to the next equation, the student positioned the arrow on the continue symbol ("<cont>"). A series of instructions and comments on the use of the paddles is given before the display appears. This series may also be accessed as an option in the "review" list (Page J). If there are no paddles connected the equations are simply displayed in order.

The essential purpose of this display is to illustrate the interdependence of the strength of the magnetic field and frequency of radiation, which represents the energy difference between the two states. Notice that the diagram in Figure 3.1 does not attempt to reflect the linearity of

the relationship between field and frequency. The diagram is intended to indicate only that two energy levels arise from a spin of one half.

The final equation on Page C is the most important and is repeated on later pages and again in the guise of question six at the end of the program.

Page D ("Transitions between States") combines the information of the previous two pages. Animation is used to show energy, as radiation, being absorbed and "flipping" the spin of the nucleus (Figure 3.3). The frequency of this radiation is again related to the type of nucleus (as represented by the gyromagnetic ratio) and the field.

Closer attention is drawn to the meaning of "the field" on Pages E and F ("Introduction to Chemical Shift" and "Formula and Derivation of Chemical Shift"). The idea that nearby electrons create a small magnetic field which modifies the field experienced at the nucleus is raised and then expanded into a definition of Chemical Shift. The necessity of having a reference compound (commonly tetramethylsilane) is stated and an equation relating frequency of signal from the sample is given. This equation has an interactive facility similar to those on Page C (Figure 3.4). A simple derivation of this formula is available if required.

Page G ("Factors influencing Chemical Shift") offers a summary of the previous pages in a single statement: "Chemical Shift is a function only of nucleus and environment". In addition the advice that "the basic Chemical Shift, for cases involving ^{1}H and ^{13}C nuclei,

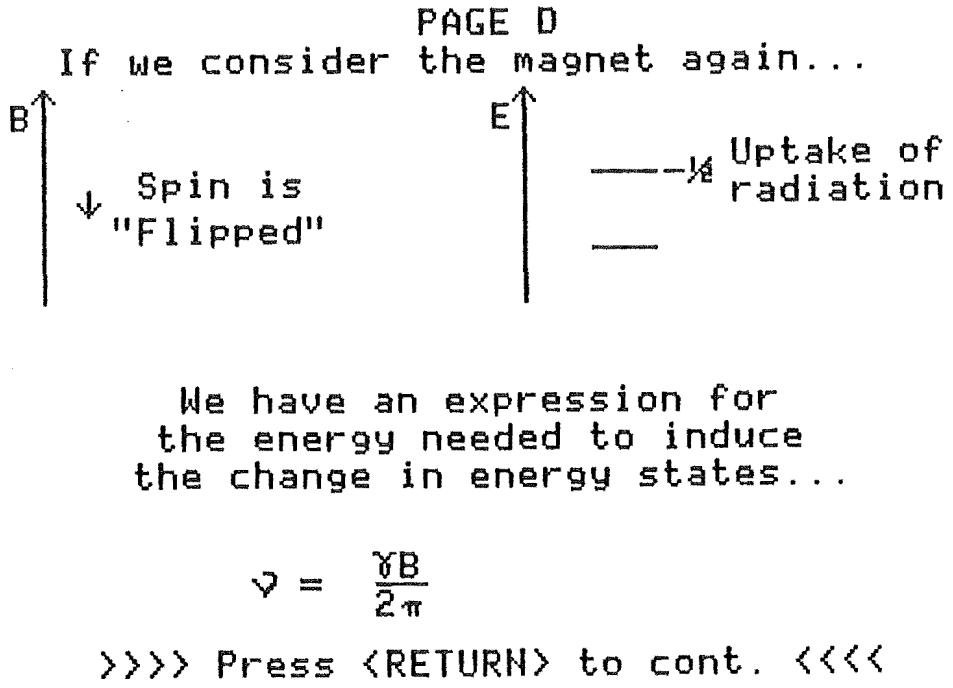


Figure 3.3

Screen images illustrating the change in energy state

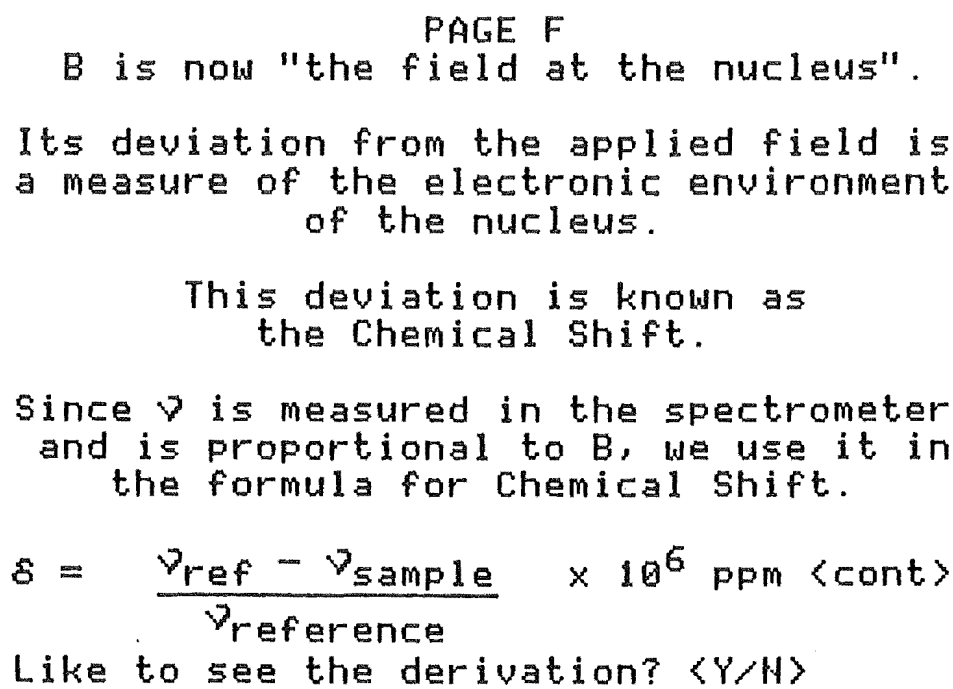


Figure 3.4

Detail of "Page" F

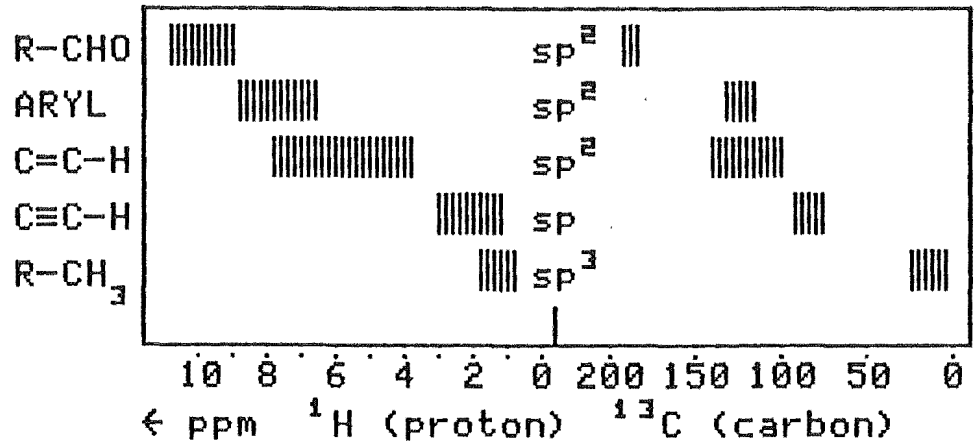
arises from the hybridisation involved" is given. Students are presented with the fact that the sp^2 hybridisations result in generally higher Chemical Shifts than sp hybrids which, in turn, generally have higher Shifts than sp^3 hybrids. The hybridisation is of the carbon atom in the case of ^{13}C NMR, and of the atom the proton is attached to in ^{1}H NMR.

Page H has a further illustration of the effects of hybridisation (Figure 3.5). In keeping with the desire to miminise both the amount and complexity of material, it was decided to limit the presentation of the relationship between hybridisation and Chemical Shift to the minimal level indicated. It became obvious during testing (Chapter VII) that this was one of the least well-remembered sections of the lesson. The importance of adequate presentation and, perhaps more significantly, of reinforcement is underlined in this instance, as there is no review of this material per se elsewhere in the package.

The concept of deshielding, the increase in Chemical Shift due to a decrease in electron density at the nucleus caused by a nearby electronegative group, is introduced, with examples, on Page I (Figure 3.6).

The seven questions accompanying PART1 briefly covered the following topics: 1) the values of nuclear spin I, 2) the number of M_I values for any I, 3) the selection rule for the change in M_I, 4) the value of nuclear spin for ^{1}H and ^{13}C, 5) the common reference compound, 6) the meaning of the symbol "δ" and 7) the meaning of deshielding.

The graph below gives an indication of the chemical shifts of the three hybrids involved.

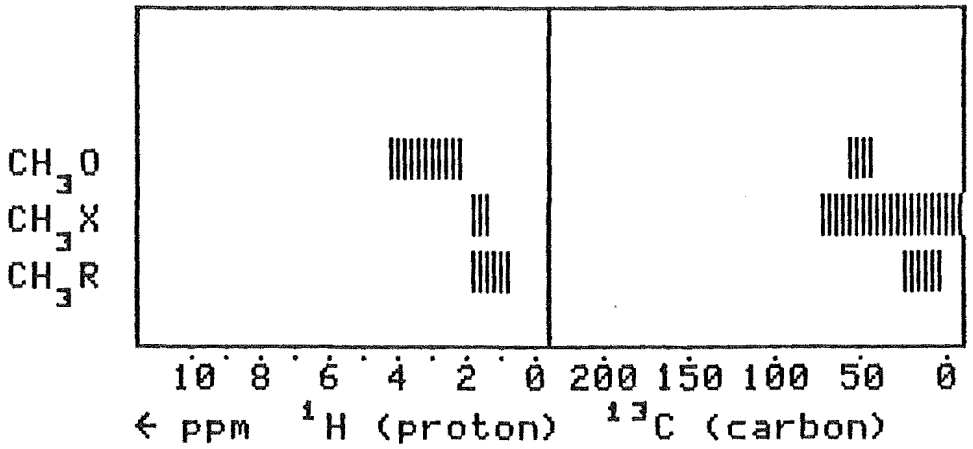


>>>> Press <RETURN> to cont. <<<<

Figure 3.5

Effect of hybridisation on Chemical Shift

Notice the changes caused by an electronegative group, such as oxygen (R is an alkyl group, X a halogen).



>>>> Press <RETURN> to cont. <<<<

Figure 3.6

Effect of Electronegativity on Chemical Shift

As previously mentioned, the purpose of the questions was not for testing, but rather was for the presentation of material again in a different form. Both the style and emphasis was changed from that of the main program, but the intent was basically the same, to encourage understanding as far as possible. To facilitate and enhance the presentation of questions, a language based on that used on the mainframe was developed. More detail on this language, called MASTER, appears in Chapter V, and the questions for the Tutorial programs are detailed in Chapter VI.

3. THE SECOND TUTORIAL PROGRAM

As with PART1, it was decided to start PART2 with an Introduction, with a similar message about the use of the ESC key to access the review/preview facility. A similar list of descriptions of the pages was available to students. The list was:

A. Review of Chemical Shift,
B. Introduction to Coupling,
C. Important factors in Coupling,
D. Chemical Equivalence and Range,
E. Differences between ^{1}H and ^{13}C NMR,
F. Coupling in CH (^{13}C),
G. Coupling in CH_2 (^{13}C),
H. Coupling in CH_3 (^{13}C),
I. Review of Pages A to H,
J. Closer Study of the Spectra of Ethanol,
K. Detail of the Coupling involved,
L. Analysis of its ^{13}C Spectrum,

M. Analysis of its ^{1}H Spectrum,

N. The Integration Line,

Q. The Questions,

X. Exit and return to the main menu.

Having judged the concepts involved in Spin-Spin Coupling to be more difficult for students, it was decided to present the material in terms with which they would be quite familiar. The common compound ethanol was widely used as an example throughout the program. While there were some complications arising from this decision, for example the awkward OH resonance in the proton spectrum (with its variable appearance and Chemical Shift), further discussion of these very complications was able to be introduced naturally.

Page A introduces the proton spectrum of ethanol, based only on Chemical Shift, and briefly reviews the most important feature, which was that the difference in Chemical Shift of the two types of proton results from the proximity of the electronegative oxygen atom.

On Page B a parallel is drawn between the effect of nearby electrons (resulting in Chemical Shift) and that of nearby nuclei. It is noted that this effect is referred to as Spin-Spin Coupling.

The important features involved in Coupling, chemical equivalence and distance, are given on Page C. Using the example of ethanol the various types of equivalence are examined. More complex examples including cyclohexane and benzene are also included.

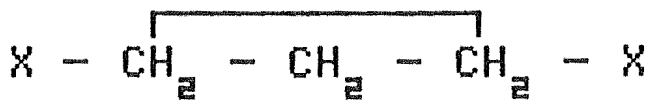
The mainly textual material of the preceding pages is clarified and expanded upon on Page D ("Chemical Equivalence and Range"). Using part of a straight chain molecule, $X - CH_2 - CH_2 - CH_2 - X$, the equivalent and then non-equivalent groups are indicated. As it is mentioned, each CH_2 fragment is illuminated by enclosing it in a "box" and "flashing" it, while computer-generated sound provides further emphasis. The groups in question are connected by a line in order to make the screen display meaningful once the dynamic illustration is complete (Figure 3.7). Range effects for proton NMR are explored in a similar fashion.

Page E indicates that there are differences between ^{1}H and ^{13}C NMR in terms of coupling. Students are informed that homonuclear coupling is of minor importance in ^{13}C NMR (unlike proton NMR) and heteronuclear coupling between ^{1}H and ^{13}C is of major importance. In keeping with the desire to avoid possible distractors, the terms "homonuclear" and "heteronuclear", although descriptive, were avoided. Mention of the term "decoupled" was made on Page E, although not in a strictly accurate sense. A rudimentary idea of decoupling was given in succeeding Pages and this concept was further explored in another section of the package (Chapter VI).

Pages F, G and H all deal with coupling arising in ^{13}C NMR in CH, CH_2 and CH_3 groups respectively. For two major reasons this approach was preferred to that of using a variety of alkyl halides (such as 1,1,2 trichloro-ethane) and studying their proton spectra.

PAGE D

For the case of ^{1}H NMR
consider the following molecule:
(both X's are identical)



THIS methylene group...
is chemically equivalent to ...
...THIS methylene group.

>>>> Press <RETURN> to cont. <<<<

Figure 3.7

Dynamic illustration of Chemical Equivalence in PART2

Firstly, it was thought necessary to dispense with possibly confusing and bewildering compounds, as the concepts had proved difficult enough to master. Secondly, there was a desire to make the use of ^{13}C NMR seem commonplace. This last intention was seen to have been somewhat justified (Chapter VII). On the three Pages in question (F, G and H) the various combinations of nuclear spins are shown and the resulting coupling patterns displayed.

A short summary of the new information followed by the statement "n neighbouring nuclei give rise to n + 1 peaks in the multiplet, with ratios according to Pascal's triangle" is given on Page I. The fact that this "rule" is only valid for first order spectra is not given here, but is left to a later stage in the teaching package as with some other previously-mentioned details.

More detailed analysis of the ^{13}C and ^{1}H NMR spectra of ethanol begin on Page J, with a short preview and the display of the spectra.

Page K (Figure 3.8) was regarded by many users as the highpoint of this program. It contains a full analysis of the source of the coupling in ethanol. For the case of ^{13}C NMR, firstly the carbon of the methyl group is chosen as the centre of interest. The four nuclei bonded to it are indicated using a sound-augmented, visual display. One of these four nuclei, the methylene carbon, can be said to have a zero nuclear spin (due to the low natural abundance of ^{13}C, which has a spin of 1/2) and so the methyl carbon has three nearby, non-equivalent nuclei with non-zero spin (the three protons). The presence of a quartet in the spectrum

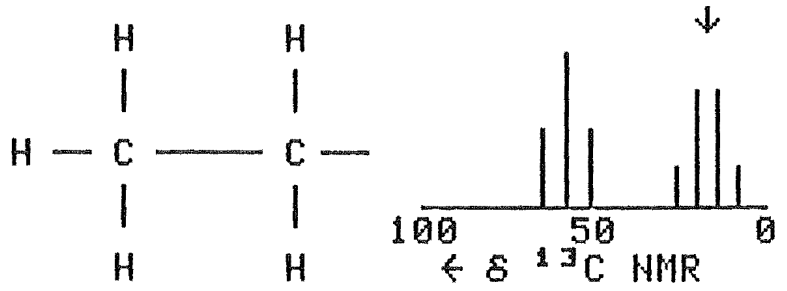
is predicted and the spectrum is displayed with the quartet being vigorously indicated. Similar animated displays are used to complete the analysis for the methylene carbon and then (optionally) to perform an analysis of the proton spectrum of ethanol.

Analysis of the spectra from the opposite point of view, deducing the compound from the spectrum, is conducted on Pages L and M. The number of different carbons in the molecule is deduced from the number of multiplets on Page L. Assigning the multiplets, first by Chemical Shift and then by coupling pattern, follows. A similar analysis is performed on the ^{1}H spectrum on Page M, with the added discussion of the reasons for the omission of the OH resonance. This was because it was thought that students would be familiar enough both with the spectrum and with the idea that there was a difference between the OH proton and the alkyl protons.

Page N continues with the proton spectrum and has brief notes on the use and value of the Integration Line (Figure 3.9).

The seven questions appended to PART2 are somewhat more testing than those of PART1, although they were enthusiastically received by students. There was more emphasis placed upon illustrating points of doubt displayed by students. The observed tendency for students to review material after scoring badly was an indication of success.

The questions covered the following areas: 1) where Chemical Shift arises from, 2) Chemical equivalence, 3) the factors involved in coupling, 4) differences between ^{1}H



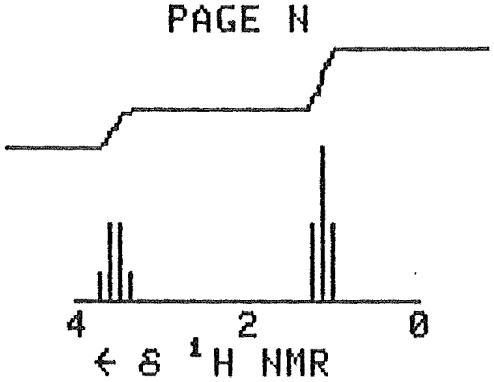
The carbon has 3 nearest neighbours
** WITH I > 0 **
and so the peak representing it
appears as a QUARTET....

(I hope you remember that
n neighbours cause n+1 peaks --> Page I)

>>>> Press <RETURN> to cont. <<<<

Figure 3.8

Analysis of ^{13}C NMR spectrum of ethanol



As it is very helpful to know this ratio
for the various peaks,
an INTEGRATION line is included.

>>>> Press <RETURN> to cont. <<<<

Figure 3.9

The integration line in a proton spectrum

and ^{13}C NMR spectra, 5) the number of peaks arising from n neighbours, 6) the ability to distinguish ^{1}H and ^{13}C spectra and 7) the Integration Line. Further detail on the Questions associated with PART2 is given in Chapter VI.

4. SUMMARY

The Tutorial programs formed the heart of the teaching package. Because of the manner in which the information had been organised and presented these programs ensured that the basic information on NMR was freely available. The programs themselves are not easily adaptable to other teaching areas, being straight PASCAL programs, but this was not unexpected. Nevertheless of major importance are the ideas and approach embodied within them. There are apparently few topics in Chemistry which would not be suitable for presentation in the manner of these Tutorial programs.

It is perhaps inevitable that this tutorial style will be compared to other educational methods, especially text books. Such a comparison, made per se, would be unfortunate. Computer Assisted Learning exercises are not intended as competition for the more traditional teaching methods. Rather the two approaches are complementary as a comparison makes clear.

As has been indicated the material for the tutorial programs was distilled from a wide range of textbooks and lecturers, and was tailored to the needs of the students for whom it was intended. In addition the nature of the programs demanded that the information be clearly and carefully presented. Cronbach (1963, p.416) noted that

these qualities are only found in superior textbooks. Textbooks are typically intended to present material upon an entire subject. Since limits upon the amount of space used in the presentation are not usually a consideration and since readers have the freedom to review previous pages, textbooks do not need to depend upon a clear and carefully-structured presentation to the same extent. Hence where textbooks offer coverage of an entire topic, a CAL package offers instruction on specific and relevant parts of a topic.

The volume of material contained in any text book is, at present, much greater than that of any teaching package and is available at rather less cost. This, however, may change in future and, for this reason, it was felt necessary to place some emphasis upon the presentation of structured information during a Computer Assisted Learning exercise.

Part of the assessment process of the tutorial programs involved their inclusion in CAL laboratory classes, as has been previous described (Chapter I). Two groups of students, those who had used the tutorial programs and those who had not, were compared in their use of the mainframe CAL exercises. The users of the tutorial programs (which were not entirely completed at the stage) completed the "test/teach" program faster, scored highly enough to reach the second part of the program at the first attempt and generally had fewer questions about Chemical Shift and Spin-Spin Coupling than their classmates.

Of interest was the difficulty that students had with one question of the mainframe exercises: "What does the

symbol Y stand for in the equation: F = G * Y / 2 * (PI) ?". The way in which the equation was displayed arose from the limitation of the teletype terminals upon which the "test/teach" program was based. Almost all of the students who had used the tutorial programs first failed to recognise this equation as being that in Figure 3.2. Certainly this was indicative of the limitations of a teletype display.

CHAPTER IV

ANALYSIS AND SIMULATION OF NMR SPECTRA

Having reached a stage at which the background material was available for study (Chapter III) it was felt that students should be given the opportunity to explore and test their knowledge. The direct cognitive style used in the tutorial programs was changed to an approach based on acquiring an intuitive feeling for the quantities involved by experiencing them in an affective environment. For example, the repeated observation in the course of analysing several proton NMR spectra that methyl resonances appear at a Chemical Shift of about 1 ppm, would have a greater impact than a series of statements to the same effect.

The two major ideas presented in the tutorial section, Chemical Shift and Spin-Spin Coupling, provided the obvious areas on which to base experimental exercises. In accordance with accepted conditions for active practice effect (Cronbach, 1963, especially p.283-304), it was decided to maximise the resemblance between these exercises and tasks routinely performed by students. Since the teaching package was likely to be used in conjunction with laboratory sessions, it was therefore decided to base the exercises on the analysis and prediction of NMR spectra, which were common laboratory tasks.

From a technical standpoint it is usual to use a simulation style of programming (Chapter I) when the

interactions and workings of various factors are being studied. The initial idea envisaged the production of a program which would calculate and display the spectrum of a molecule input by the student user. The molecule would be entered as a series of fragments each accessed by a single keystroke from a short list appearing on the screen. Upon completion of the molecule the proton spectrum would be calculated and displayed.

When this was implemented limitations concerning the range of fragments and more particularly how they could be interconnected, meant that students could not always enter the molecules of their choice and often quickly surpassed the capabilities of the program. While sometimes amusing, exposing the shortcomings of the program was not very helpful to students. Even so reactions to the exercise were very positive. Comments ranged from very general, "I love it" and "It's really amazing", to more specific confirmations of success: "I can really get into this now. It's not really hard when you get into it!".

Observations on how students used the program indicated the need for further expansion of the teaching package. Having obtained a spectrum, students invariably attempted to assign the resonances to the various parts of the molecule, as was intended when the program was designed. However the methods that the students employed were often not ideal and sometimes resulted in incorrect analyses. That this behaviour was undesirable was obvious: "if a person practices before he knows the correct general pattern of the task, he is likely to practice the wrong

actions" (Cronbach, 1963, p.284). Design of an exercise to help students analyse proton spectra was therefore necessary.

One of the major reasons for not developing an analysis program earlier was the existence of such a program implemented on the mainframe computer, program "S201" in Ayscough, Morris and Wilson (1979). With the establishment of the need for such an exercise as part of the present package it appeared sensible to base the approach upon that embodied in the moderately successful mainframe program, at least in the early stages of development.

The analysis of a proton spectrum should lead to the deduction of the structure of the compound given only its basic formula. Each resonance is examined in turn. The fragment of the molecule is identified using the Chemical Shift and number of protons (deduced from the integral) and then information about the fragment's neighbours is obtained from the coupling pattern and Chemical Shift. When all of the resonances have been examined the fragments are connected in accordance with the given formula.

The strategy used in the mainframe program was simplified and from this an analysis exercise was constrcted and incorporated into the teaching package. This simplification, added to the fact that the strengths of the microcomputer were utilised (mostly in the graphics field), meant that the final result bore only superficial similarities to the original. Details appear in following sections.

relaxation of some of the constraints on construction, a representation of the molecule being entered on the screen and a demonstration of how to use the program.

Student response to the two programs was very satisfying. In a typical session a student would use the analysis program to study two or three spectra, gaining some expertise, and then switch to the simulation program. Here spectra of increasing complexity were created and analysed using the newly learnt techniques. That this was the case represented a striking indication of successful planning and implementation in the teaching package. In addition, publication of the programs (Draper and Penfold, 1984) received encouraging responses from other CAL authors.

1. THE SPECTRUM ANALYSIS PROGRAM

The analysis program, NMRSPEC, was produced primarily with the aim of giving students the opportunity to practice analysing spectra. Continued exposure to typical Chemical Shifts and coupling patterns was, as previously indicated, also a major underlying aim. It was intended that the program be used to complement the simulation exercise described in a later section.

(1) Outline

In NMRSPEC, the strategy for "solving" spectra involved the deduction of as much information as possible about each resonance in turn. For each singlet resonance this involved the deduction of a fragment of a molecule from the integral, with Chemical Shift or Coupling pattern being

this involved the deduction of a fragment of a molecule from the integral, with Chemical Shift or Coupling pattern being used in cases of confusion. Detailed consideration of the Chemical Shift then gave information on neighbouring groups, with the coupling pattern or molecular formula being used where helpful.

Consideration of the multiplet peaks was made after the singlets in the interests of simplicity, since the multiplets have an intermediate step. This extra step involves the deduction of neighbouring groups from the nature of the coupling, using the first order rule (n protons as part of non-equivalent neighbouring groups result in a couplet of n+1 peaks for that resonance).

Having analysed all of the resonances the structure of the compound was deduced by establishing the correct connectivity of the fragments. In fact for each of the spectra the solution was unique once the analysis was completed.

Involving students in complicated interactions with the computer was thought not only to be unnecessary in this exercise, but also to be a possible distraction from the objectives. For this reason it was decided to require only single keystroke input from students. To facilitate this short lists of options labelled with numbers, known as "menus", were used throughout (Figure 4.1). Furthermore the amount of text to be read on the screen at any one time was limited to one or two short sentences.

With considerable emphasis being placed on deduction of information from a set of data, clarity and simplicity of

as a series of vertical lines (Figure 4.2) rather than as a more realistic approximation. Each singlet or multiplet resonance was labelled for ease of reference.

In order to enhance student appreciation of Chemical Shift it was decided to draw all spectra on a constant scale. Therefore, irrespective of the rest of the spectrum, resonances of groups with chemically equivalent environments (i.e. having similar Chemical Shifts) would appear at the same screen position. Expansion of the scale so that the spectrum of a molecule utilised the entire screen (for example Palmer, 1981) was thought to distract from the objective of obtaining an overall view of the relative positions of the resonances. Having a constant scale was an important step in maintaining the realism of the program. For example a resonance appearing at the right hand side of the screen implied that the Chemical Shift value was low and hence was possibly a methyl group attached to an alkyl group. The overall position of a resonance with regards to the Chemical Shift scale is maintained as it is in a series of actual spectra.

From the student viewpoint the object of the exercise was the deduction of the structure of a compound. It was therefore important that there be an effective means of entering that structure as an answer. As has been previously stated this exercise was not designed to be a test of student ability to communicate with the computer.

Here is a list of common fragments:
1> CH_3 2> CH_2 3> CH 4>  5> OH
Suggest a fragment for peak 2
(note the number of protons is 3)

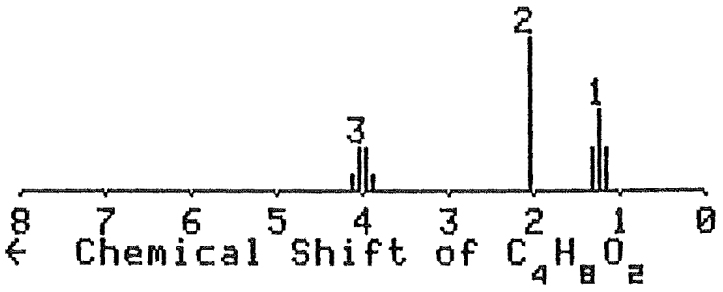


Figure 4.1

Menu input in NMRSPEC

Press <SPACE> to continue
In this molecule we have 8 protons
and so we can deduce the ratio to be
2 : 3 : 3

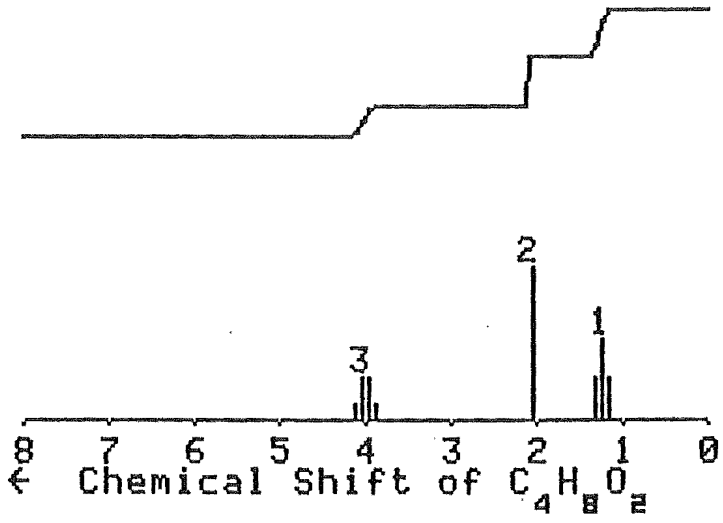


Figure 4.2

A spectrum displayed in NMRSPEC

Thus entering fragments from a list to construct the molecule for example, was considered unsuitable. Similarly a "free format" approach, with the student submitting the complete structure in words (or formulae) was rejected primarily because of the risk of error involved in judging the response. A student answer labelled incorrectly would considerably undermine the purpose of the exercise. Problems arise from the number of different ways of entering the structure for even a relatively simple molecule such as ethylacetate (e.g. $CH_3COOCH_2CH_3$, $MeCO_2ET$, ethyl acetate, ethylacetate, etc.). Even so these are much less than the difficulties associated with incorrect responses. Replies such as "No, that is incorrect" were considered to be of little value. More meaningful replies were required.

An added complication was the fact that the program was constructed with an expandable database, with a suite of accompanying utility programs designed to make additional spectra available. It was not considered reasonable to expect the CAL Author to allow for all possible answers (correct and incorrect) for the molecule for the new spectrum. Student entry of the structure of the compound was therefore made into a simple multichoice exercise, with incorrect selections receiving useful comments. This style was judged to be consistent with the remainder of the program and simplified the task of the teacher, although requiring some technical expertise with graphics.

(2) A Sample Run of NMRSPEC

Upon the commencement of the program a short introduction is presented, apparently with the intention of

providing some instructions about the use of the program and some reminders about the theory. Although this was indeed a consideration, the introduction served another function. It was apparent that instructions at the beginning of an exercise such as this were not very carefully considered and even less well-remembered by student users. The initial screen display was constructed as an enhancement of the program, in that it makes the considerable amount of preparation (commonly known as initialisation) that must be completed before the user can begin, rather less obvious. On a small computer, such as the microcomputer used in this research, transfer of large amounts of data usually means lengthy delays, which can seriously damage the credibility of a teaching exercise. Throughout the teaching package are examples of attempts to conceal the internal workings (which are usually limitations) of the computer from the user, who should not be burdened with such detail. In NMRSPEC the amount of attention given to the initial instructions made no difference to the usability of the program.

The first task for the student is to choose a compound from a displayed list of empirical formulae (Figure 4.3). Up to twenty compounds with their associated spectra may be included by the teacher. Nine fairly simple compounds are included in the teaching package.

The spectrum of the compound is then displayed and the student asked if the "integration tutorial" is required. This brief series of statements reviews the relationship between the area occupied by each resonance and number of protons it represents. It also details how changes in

Please choose a compound:

A> $C_4H_8O_2$
B> C_8H_{10}
C> C_7H_8O
D> C_9H_{12}
E> $C_{10}H_{14}$
F> $C_6H_{12}O_2$
G> $C_6H_{10}O_2$
H> $C_7H_{12}O_4$
I> $C_3H_7NO_2$

Which Spectrum? (letter) >

Figure 4.3

List of available compounds in NMRSPEC

height of an integration line are therefore proportional to the number of protons. An integration line is drawn and the number of protons deduced for each resonance (Figure 4.2).

A table of data for the spectrum, containing Chemical Shift, number of protons and multiplicity of each resonance, is available to the student. This information is obtained by pressing the "ESC" key as instructed. In order to ensure that this has been understood students must press the correct key (and therefore view the data) before proceeding.

Analysis begins by considering the singlet resonances. Choice of the most appropriate fragment of the molecule is made from a short list by considering the number of protons (Figure 4.1). Brief comments on incorrect selections are displayed.

Consideration is then made of the Chemical Shift in more detail. A diagram is presented, showing the ranges of Chemical Shift values of the particular fragment with a variety of neighbouring groups. At this point a question offering an explanation of the meaning of the symbols and the purpose of the display is presented by the computer. A similar question is posed each time the diagram is presented until the explanation has been seen or the spectrum has been successfully analysed. From then the question is posed only when the first fragment of a new spectrum is being considered. Various strategies of making the explanation available were considered and evaluated. These ranged from a compulsory display of all instructions to none at all. The final solution left the choice of receiving instruction

firmly in the hands of the user, who is obviously the best judge of whether it is needed.

The Chemical Shift of the fragment under inspection is indicated as a vertical line (Figure 4.4). This allows the neighbouring group to be deduced from the intersection of the shift line with the range of shifts for the particular types of neighbours. Occasionally factors such as the coupling pattern or formula of the compound are needed to separate alternatives. In the example illustrated (Figure 4.4) the typical shift values of methyl groups are shown, with the shift value intersecting two groups (choices 2 and 4).

Of the six "neighbours", three need some explanation. The "CR_3" and "CR_2Z" groups are parts of a molecule based on a carbon atom with two or three alkyl groups attached. Typically at least one "alkyl" group is a proton, which means that the extent of coupling between this possibility and the fragment under investigation can be used as an aid. In fact in the example (Figure 4.4) neighbour "2" is rejected as a possibility, since there is no coupling of the CH_3 group resonance. Examples of "CR_3" are CH_3 and $CH(CH_3)_2$ and of "CR_2Z" are CH_2O and $CHCH_3Cl$. A "Z" group is any electronegative group, usually options 3, 4 or 5, while a "Y" group is any electronegative group not already in the list, with typical examples being Cl, Br and NO_2.

The possible choices in Figure 4.4 are neighbours "2" and "4" by Chemical Shift and, as has been indicated, choice "2" is eliminated on the assumption that it would cause some coupling (i.e. at least one of the "R" groups is a proton).

Following this display is a summary of the information obtained so far (Figure 4.5) and an opportunity is given to determine the structure of the compound. Only one attempt at the structure is permitted: an incorrect guess returns the student to the spectrum for further analysis.

Analysis of the multiplet resonances involves the added study of the coupling pattern, which is an aid in the determination of neighbouring groups. The simple first order rule ("n neighbouring protons give rise to n+1 peaks in the multiplet") is used to find the number of protons in the neighbouring groups and this is related directly to structural information. One, two and three protons are taken to imply CH, CH_2 and CH_3 respectively, while four protons represents two CH_2 groups, five a CH_3 and a CH_2 and six protons two CH_3 groups.

If the student cannot deduce the number of protons from the multiplet, the general rule is available as a hint. Upon failing for a second time the student is given the correct answer and the relevant structural information (Figure 4.6).

Having analysed all of the resonances the information is fully summarized and the student is expected to combine that information and to deduce the structure of the compound. In all cases the full summary of information leads to a unique structure. Figure 4.5 shows an example of a summary. Three statements, one for each of the resonances, review the information that has been deduced in the analysis. The neighbour responsible for the particular Chemical Shift is indicated ("CH_3 shift from C=O") and,

Which neighbour to CH_3 do you think?
(The formula is $C_4H_8O_2$)□

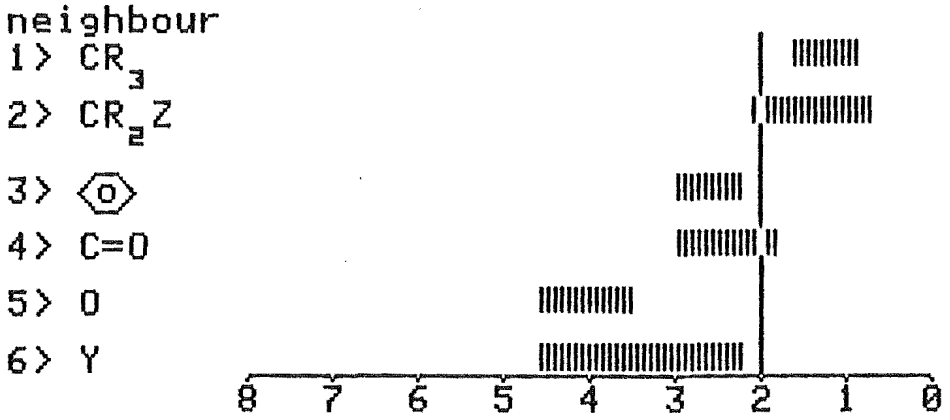


Figure 4.4

Deduction of a neighbouring group by Chemical Shift

Press <SPACE> to continue
So far we have seen the following...

CH_3 shift from CR_2Z split by CH_2

CH_3 shift from C=O

CH_2 shift from O split by CH_3

Try to connect these fragments up
so that a molecule is formed...
(The formula is $C_4H_8O_2$)

Figure 4.5

Summary of information for a spectrum

where relevant, the neighbouring groups causing the coupling are indicated.

As has been indicated entry of the final structure by the student is another menu choice (Figure 4.7). Usually four possible structures are given, with typical distractors being isomers (molecules having the same fragments, but connected differently) and molecules with similar spectra to the correct answer but with different formulae. Where an incorrect answer is entered an explanatory comment is given (Figure 4.7). Upon entering the correct answer the student has the opportunity to analyse more spectra.

(3) The Teacher's Part in Spectrum Analysis

The analysis program was constructed with teachers, as well as students, in mind. It was intended that the selection of spectra be determined by individual teachers who would be able to select those most appropriate to their needs. A maximum of twenty at any time was allowed for, the limiting factor being the number of formulae which may be displayed on the screen simultaneously (Figure 4.3).

A separate program was written to allow easy creation of spectra (Appendix A). It did not however allow their removal. This was because the simplicity of the approach used in the analysis program did not allow a unique solution for all parts of the analysis. The spectrum of diethyl malonate ($C_7H_{12}O_4$), for example, has one resonance (the singlet CH_2) resulting from a fragment whose neighbours cannot be uniquely identified by Chemical Shift alone. They may only be deduced when the other resonances have been considered. This fact had to be "hard coded" (explicitly

Press <SPACE> to continue
For a multiplet of 4 peaks
how many protons must there be
on adjacent carbon atoms [1]
No.....
The answer is 3,
So we can deduce CH_3
next to the CH_2 group.

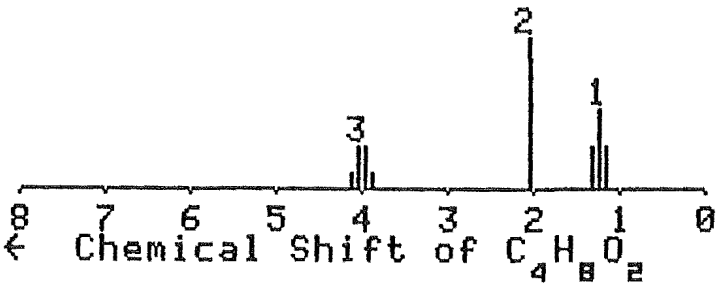


Figure 4.6

Deduction of neighbouring group from coupling

Press <SPACE> to continue
Choose the structure of the compound:

1) $CH_3-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$

2) $CH_3-\overset{\overset{O}{\|}}{C}-CH_2-O-CH_3$

3) $CH_3-CH_2-\overset{\overset{O}{\|}}{C}-O-CH_3$

4) $CH_3-\overset{\overset{O}{\|}}{C}-O-CH_3$

Input your choice (a number) > [3]
A CH_3 and the CH_2 have wrong shifts,
although the splitting pattern is right

Figure 4.7

Entry of the structure of the compound

written into the program), which meant that complications could arise if existing spectra were able to be removed. Similar hard-coding would be required for analogous non-resolvable conflicts for teacher-entered spectra. The process of creating a new spectrum is designed to be as simple as possible. Once the formula is given, information about each resonance in turn is requested and consists of three parts: the fragment responsible for the resonance, the neighbouring groups and the Chemical Shift of the resonance. The choice of fragments is made from menus in a similar fashion to NMRSPEC.

As with the analysis program, determination of how the structures associated with the spectrum were to be entered proved to be a difficult problem. In an early version the teacher was required to enter each structure as a linear series of fragments which could then be converted into a display. The results of this method were seldom wholly satisfactory however. The eventual solution was to request the teacher to create a complete graphics screen with four possible structures on it. For each structure the teacher would enter suitably meaningful comments to be displayed when students selected the particular structure. The tools for creating and storing the screen display are described in Appendix A. The nature of the task meant that the teacher needed some experience in editing screen displays.

A more satisfactory alternative might have been a combination of both of the above methods into a limited "graphics editor". The teacher would then have been able to create a graphics screen by choosing fragments (from a menu)

and positioning them, perhaps with the aid of a joystick. An acceptable display could therefore be formed without the need for technical knowledge.

2. THE SIMULATION PROGRAM

The underlying concept of the simulation program, NMRSIMUL, was simple. The user enters a molecule and an approximation of its proton NMR spectrum is displayed. This spectrum is derived from general principles and tailored to the data from the spectra used in NMRSPEC.

The two major factors influencing proton Chemical Shift are the basic type of fragment and the effects of neighbouring groups. In setting up the internal data each proton-bearing fragment of a molecule was given a Chemical Shift which was then modified by considering the adjacent groups. One exception was the benzene nucleus, whose Shift was defined to be unaffected by neighbouring groups. The complete spectrum of a molecule can therefore be deduced by analysing each fragment in turn. Table 4.1 contains the fragments and their appropriate values and also contains examples of the values calculated for two compounds ($C_2H_5OCOCH_3$ and $CH_3C_6H_4CH(CH_3)_2$).

The above method is, of course, rather limited. A benzene nucleus is assumed always to give rise to a singlet resonance at a Chemical Shift of 7.2 ppm irrespective of its environment. This simplicity is, however, in keeping with the aim of the exercise. Adding complexity to give a more exact value of Chemical Shift and more realistic spectra would have served little purpose as the program was not

Table 4.1

Data for NMRSIMUL

Values used in the construction of spectra

	Fragment	Bonds left to be formed	Basic Shift	Modifying Shift
1	CH_3	1	1.1	0.1
2	CH_2	2	1.6	0.2
3	CH	3	1.9	0.2
4	CO (carbonyl)	2	-	0.9
5	O (ether)	2	-	2.0
6	Benzene nucleus	1 (2)	7.2	0.9
7	Cl	1	-	1.9

Examples of calculated shifts values

	Fragment	Shift Actual	Shift Calculated
$CH_3CH_2OCOCH_3$			
	CH_3 (ethyl)	4.1	3.7
	CH_2	1.2	1.3
	CH_3 (methyl)	2.0	2.0
$CH_3C_6H_4CH(CH_3)_2$			
	CH_3 (toluyl)	2.2	2.0
	C_6H_4	7.1	7.2
	CH	2.8	3.0
	CH_3 (alkyl)	1.1	1.3

intended to be a precise analytical tool. As illustrated (Figure 4.8) the spectra produced by the program approximate the actual appearance in terms of position and shape.

Coupling follows the first order rule: n non-equivalent protons in neighbouring groups produce a couplet of n+1 peaks. Equivalence of neighbouring protons is simply assessed; with neighbouring protons deemed to be equivalent if they are part of the same type of fragment and their Chemical Shift values are identical.

The discrepancies between the spectra used in the simulation program and the actual examples students would encounter were not forgotten however. The question of the supply of a bridge between the teaching package and the realities students would face was given considerable attention and is addressed at a later stage (Chapter VI).

(1) Techniques used in the Simulation

Ease of use was considered to be of major importance for this section of work and so, as with the analysis program, student interaction with the computer was designed to be simple. Only single key strokes are needed and the list of valid keys is displayed in the previously described "menu" style (Figure 4.9). To enter any fragment a student has only to press the appropriate number key (listed in Table 4.1).

Two other keys are of some importance. The backward arrow enabled fragments to be removed and the forward arrow displayed the alternate graphics screen. Alternate graphics screens were provided so that spectra of different compounds could be easily compared.

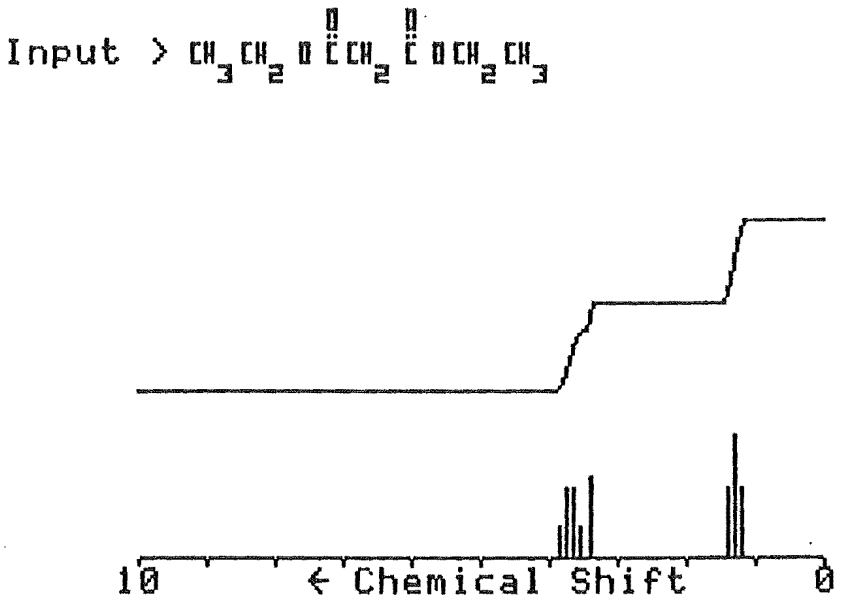


Figure 4.8

Simulation of the spectrum of diethylmalonate

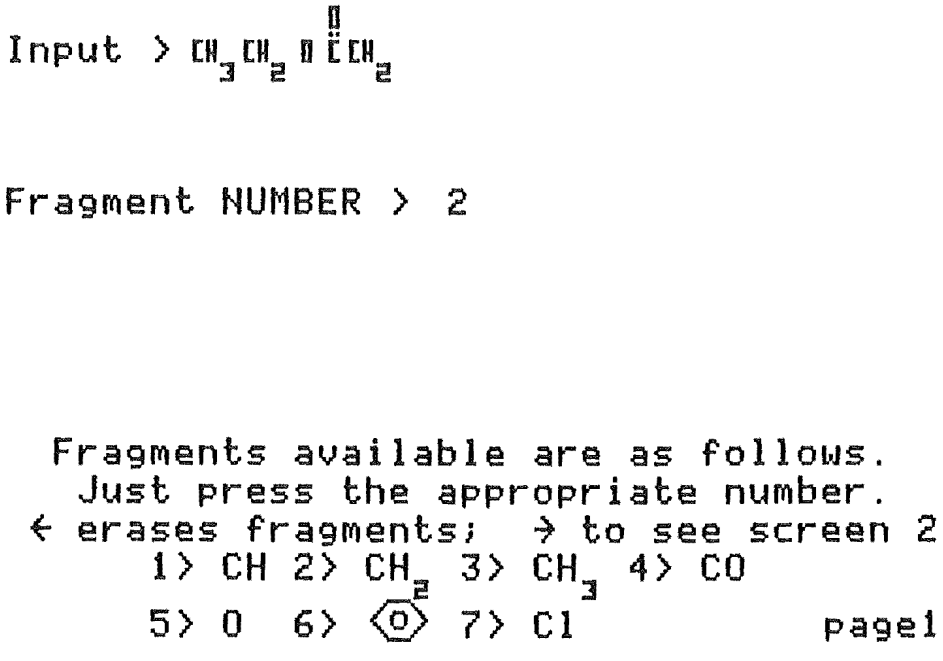


Figure 4.9

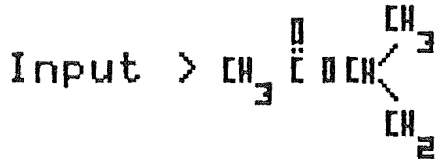
Entry of a compound using NMRSIMUL

To further enhance the effectiveness of the display, as well as to provide a record of the entries made, it was decided that a representation of the molecule being constructed should be included. As each fragment is entered its representation is added to the molecule on the screen. Requesting the removal of a fragment (using the backarrow key) results in the removal of part of the molecule.

The characteristics of the fragments affect the way in which they may be used. Two fragments, CH_3 and Cl, may form only one bond and so act as "terminators", since their entry will end a series of fragments. Benzene is also regarded as acting as a terminator. Three other fragments act as "perpetuators" of a series. These fragments, each with two further bonds to form, are CH_2, O and CO.

The remaining fragment, CH, provides two further places to add fragments after it has been added to the chain and so creates a "sidechain". In the screen display a sidechain is displayed offset slightly and above the chain from which it arose. When this chain is terminated, further fragments may be added to the molecule at an offset below the original chain (Figure 4.10). Thus if CH groups are used carelessly "collisions" between sidechains may occur. To reduce this possibility only two sidechains at a time may be in an incomplete state.

When entry of the molecule is complete, its spectrum is displayed with similar form to those of the analysis program. The display is a simple "stick" diagram and all spectra are displayed on a fixed Chemical Shift scale. This last feature is especially important due to the ability of



Fragment NUMBER > 2

Fragments available are as follows.
Just press the appropriate number.
← erases fragments; → to see screen 2

1> CH 2> CH_2 3> CH_3 4> CO

5> O 6>  7> Cl page1

Figure 4.10

Entry of a "sidechain" in NMRSPEC

the student user to construct and compare two spectra at once. If the display was tailored to the range of numerical values of the data, usefulness as a comparison would be diminished. Having a constant scale ensures that changes in Chemical Shift and coupling patterns may be seen at a glance.

A demonstration of some of the capabilities of the program was included (including some pitfalls in its use) to explain some of the procedures. A primary aim of this feature was to illustrate the actions of the various keys, in particular how to enter and remove fragments and how to view the alternate graphics screen. A suitable warning about CH groups was also included.

(2) A Sample Run of NMRSIMUL

To illustrate the sequence of events involved in constructing a spectrum a suitable compound was needed. The example chosen was diethylmalonate ($CH_2(COOC_2H_5)_2$), one of the compounds used in the analysis exercise.

At the start of the program a brief set of instructions is displayed, with a similar purpose to that of the analysis program. An outline of the various functions is offered and, as before, it also serves the useful purpose of occupying time during program initialisation.

The opportunity for a demonstration of how to use the program is then offered. This demonstration contains most of the instructions and includes a number of valuable hints for using the simulation exercise. It is designed to be realistic and yet as easy to use as possible. The display is that used to construct molecules and display spectra with

the addition of two or three lines of text containing advice (Figure 4.11).

The demonstration contains the following information. Firstly, the importance of preparation is stressed ("Write out the structure of the compound beforehand"). Secondly, an example of entering ethylacetate is given and included is the use of the backarrow key to remove a fragment. The resulting spectrum is then displayed (Figure 4.12). Thirdly, attention is then drawn to the fact that two graphics screens are in use and the action of the forward arrow key is illustrated. Fourthly, a compound isopropylacetate ($(CH_3)_2CHOCOCH_3$), is used to illustrate the effect of the CH group upon the display (Figure 4.10). The overall ease of molecule entry is illustrated throughout with the fragment number appearing, followed by the representation being added to the molecule.

The screen is then reset awaiting entry of fragments by the student user. Since the molecule is entered using a sequence of fragments much care is required in determining the correct order. For diethylmalonate the structure may be written as CH_3 CH_2 O CO CH_2 CO O CH_2 CH_3 and so the key sequence is simply 1 2 5 4 2 4 5 2 1 (Figure 4.9). When the final fragment is entered the spectrum is displayed.

The final menu display contains four visible options: 1) view screen one, 2) view screen two, 3) start a new spectrum on the current screen and 4) quit the program. An "invisible" option allows the current screen to be printed. After pressing "D" the user is prompted for further detail and is able to dump either graphics screen.

Input >

Fragment NUMBER >

A couple of points to note.
1) Write out your structure beforehand.
2) Enter it from one end to the other.

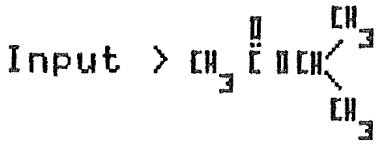
Fragments available are as follows.
Just press the appropriate number.
← erases fragments; → to see screen 2

1> CH 2> CH_2 3> CH_3 4> CO

5> O 6>  7> Cl page1

Figure 4.11

The demonstration associated with NMRSIMUL



Please press any key to continue.

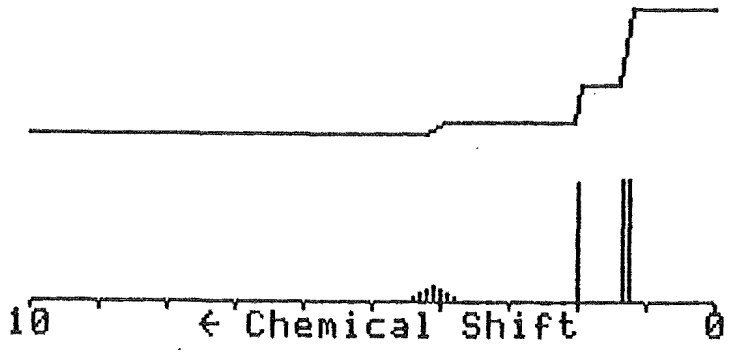


Figure 4.12

The spectrum displayed in the demonstration

3. SUMMARY

On the basis of direct observation, NMRSPEC and NMRSIMUL appeared to succeed in their aims. In a typical session a student would use the analysis program to analyse two or three spectra and then use the simulation program to enter several molecules. When making assignments the resonances in the spectra produced were invariably analysed by the student using the newly-learnt techniques in an apparently correct manner. In addition the programs were well-received by students with the most enthusiastic responses being for the simulation program. Observation of the package in use indicated that those who had used it seemed more able to analyse spectra effectively and had more appreciation of Chemical Shift of types of molecule fragments.

Without doubt the programs served a useful and necessary function as a part of the teaching package. As has been indicated the need for practice is important in any learning environment. NMRSIMUL allowed students to exercise and investigate their knowledge. Many students used the program to compare and predict the spectra of compounds in use in various exercises and experiments in the laboratory. The program was therefore acting in a simulation mode as a virtual NMR spectrometer.

NMRSPEC had a complementary role to the simulation program and functioned in a manner analogous to that of tutorial programs, in that it provided a source of knowledge and instruction that could be referred to.

While neither program is directly applicable to other areas of Chemistry, the molecule entry section of the simulation program could have widespread use. In addition each program could be further expanded within the NMR package. Some interest was expressed for the simulation program to provide ^{13}C NMR spectra. This would be a definite possibility given that only an approximate result would be required. The analysis program is able to be superficially modified with ease and has a readily expandable database of spectra with a collection of tailored utility programs.

Chapter V

DESIGNING THE MASTER LANGUAGE

As development of the tutorial, simulation and analysis programs neared completion, the teaching package as a whole was reviewed in order to establish the direction of further investigation. There were four major findings.

Firstly, although the modular design of the package allowed individual session times to be as long as required, the multiplicity of available options confused some users. A program to display the available parts of the package, went some way towards alleviating this problem.

Secondly, the presentation of some of the material was, of necessity, over-simplified. In order to avoid misconceptions in the minds of students, there needed to be an attempt to detail and explain the nature of the approximations.

The third problem to emerge was that of lack of familiarity with computers on the part of some students. Some were rather wary of the computer and some had never previously used a computer keyboard (or even a typewriter). Accommodation of those students was therefore necessary.

Fourthly, in the programs written so far student interaction with the computer was limited to the simple menu-driven variety. Even the series of questions designed to accompany each tutorial program (Chapter III) was inadequately implemented. Problems associated in

establishing a meaningful interaction between student and computer severely prejudiced the potential benefits.

When these four problems were considered, it was concluded that it would be useful to provide improved facilities for the presentation of considerable amounts of text while still allowing for the incorporation of graphics. In addition a facility to analyse student responses in detail had to be provided to enable judgements to be made of student progress and also the appropriateness of the student interactions.

1. CHOOSING THE APPROACH

Barker and Singh (1982) note that there have been two typical solutions to the problems presented above. The first is perhaps the most obvious. For each required exercise, a separate program in the original or host programming language (in this case PASCAL) is written. The second solution has been to use a separate, specialised programming language, usually referred to as an Author language. An Author language is at a higher level than the host programming language: thus one statement in an Author language is equivalent to several statements in the host language. An example of an Author language for the APPLE computer is the PILOT language in which the author writes a lesson as a series of instructions, which are then "interpreted" (converted to machine usable form) as the program is used. The "interpreter" in this case was written in PASCAL.

There are conflicting opinions as to the suitability

of each of the solutions (for example Barker and Singh, 1983, Merrill, 1982, Nelson, 1981, and Schuyler, 1979). The direct programming approach offers the full facilities of the host language and therefore complete control of the results, but does have several significant drawbacks. Maintenance of a complete program can be difficult and time-consuming, since there is a need to recompile the entire program after making changes. Gaining an understanding of a lesson by studying a low-level program is often difficult and also there will inevitably be duplication of basic facilities such as those for accepting and analysing input, presenting text on screen and dealing with graphics.

Merrill (1982) argued, however, that the use of Author languages, can be severely limiting. He maintained that the simplicity of PILOT, for example, was "achieved by reducing the number of commands in the language". This implies that the full facilities of the computer are not being used and, in addition, "encourages novice programmers to use a mediocre strategy".

There are advantages to the use of an Author language. Each lesson consists of a set of instructions dealing more with the basis of the presentation, rather than with the details of the process. An interpreter will translate such instructions and therefore avoid the duplication of code common in the direct programming method. In addition the lesson should be easier to read and understand than a program written in a full programming language and the transfer of lessons to another machine (with, perhaps, a different version of the host language)

means that only one program (the interpreter) needs to be rewritten.

Nelson (1981) expressed satisfaction with the APPLE PILOT system apart from its somewhat slow execution speed. He recommended PILOT ahead of BASIC, FORTRAN and **Pascal** as a language for preparing CAL material. Some examples of PILOT can be seen in Schuyler (1979).

While raising valid points about the limitations and benefits of Author languages, it seems likely that many writers, whether consciously or not, were trying to find one solution, in the form of an ideal programming language, to the problems of CAL. This objective is simplistic at the very least.

Consideration of the requirements of the NMR teaching package indicated that the advantages of an Author language, in the limited role in which it was to be used, would outweigh its disadvantages.

2. CHOOSING AN AUTHOR LANGUAGE

One of the aims of this research was to produce a relatively self-contained teaching package. This implied that student users would not be required to know anything about the running of the computer or its programs. Since two disk drives were standard equipment on most of the computers in the Department, a decision was made to spread the programs in the teaching package over two diskettes, but to accommodate them entirely on these in order to remove the need for students to change diskettes. In considering the choice of a particular Author language, some thought had

therefore to be given to the amount of space required for each option.

Ironically one of the reasons that the promising Author language system APPLE PILOT proved to be inadequate, was the fact that it required that diskettes be changed during a user session. Additional reasons were the slow overall speed of the implementation and, even though written in PASCAL, a disappointing lack of user access from the PASCAL Operating system below user level.

Another Author language, STAF (Science Teacher's Authoring Facility), was considered (Ayscough, 1977). A review of this language is contained in Barker and Wilford (1985). A PASCAL implementation of STAF on the microcomputer, a direct copy of a version written for a mainframe (VAX 750), was evaluated. It had most of the advantages of the STAF language, such as a comprehensive collection of mathematical functions for example and many of the weaknesses, for instance a surprising lack of consideration for the appearance of the text. The direct transfer of mainframe STAF to the APPLE was however, not satisfactory. Since the STAF interpreter program depended upon the speed and capacity of the mainframe computer for much of its effectiveness, the transfer to the comparatively slow microcomputer meant that the speed of response was unacceptable. A graphics capability would have to be added, since the interpreter was originally written for hardcopy output and this would have imposed an additional burden on the program.

The lack of suitable software therefore implied that an Author language had to be designed. Comments of many writers, "it makes no sense to start a CAI project unless one is willing to write most of the necessary software" (Nievergelt, 1980) for example, suggested that the situation was a commonly encountered one.

3. DESIGNING THE LANGUAGE

It was decided that the Author language should be based on the general ideas embodied in the STAF language. There were several reasons for this. As has been indicated previously (Chapter IV), it is unnecessary and usually wasteful to start each new CAL project from first principles if there exists a proven technique. STAF had been used extensively on mainframe computers with success (Ayscough, Morris and Wilson, 1979). Apart from the opportunity to improve on a successful product in adapting it to the microcomputer, the existing library of STAF lessons based on the mainframe would also be available for conversion and, perhaps more significantly, authors already familiar with STAF would have less difficulty using the microcomputer version than a completely new language.

With student involvement and interest vital factors in any CAL lesson, lengthy delays and slow response times will be counter-productive. It was therefore decided that an Author language lesson would be pre-processed before being interpreted, in a step analogous to compilation. This processing would include a check for correct syntax and would convert the lesson into a form more amenable to rapid

interpretation. Although this implied a slower rate of lesson development, it alleviated many concerns associated with execution speed, i.e. response times, and had the additional benefit of requiring less disk space for the Interpreter. In keeping with many languages (PILOT, STAF), an acronym, M.A.S.T.E.R. (Microcomputer-Adapted STAF for Teaching and Educational Research), was coined. A outline of some of the details of the MASTER language appears in Appendix A.

4. DESIGNING MASTER LESSONS

There are two essential aspects to the production of a CAL lesson: the overall planning of the entire lesson and the design and implementation of the reaction to student input. The MASTER language provided the essential facilities for the second of these two aspects.

In constructing a complete MASTER lesson, the Author first designs and writes the text and then moves on to the next phase using two specific features of the language. This phase concerns firstly the analysis and conversion to executable form and, secondly, the appearance of the graphics screen.

(1) Lesson Design

All of the relevant information for a MASTER lesson must be obtained and organised before lesson writing commences. The technique developed involved firstly arranging the information into an essentially linearly developing order in general subsections, so that students

could have easy access to or be able to exit from any subsection. In each subsection, material should appear as a small number of concise statements with relevant diagrams included. Some attention should be given to the use of simple diagrams, which are able to convey maximum possible information when accompanied by the appropriate text.

Questions aimed to increase both concentration and retention appear to have been used successfully in the teaching package. In a lesson primarily intended to present material, however, over-use of questions may have a distracting effect and should be avoided. Reinforcing the key points appeared to be the most effective use of questions in a teaching lesson. If, however, the intention of a MASTER lesson was to both review some of the important material and to provide an indication of level of understanding, then a series of questions may be presented. In such circumstances, as illustrated by the questions accompanying the tutorial programs, the presentation of the complete answer is of utmost importance.

(2) Matching Responses

Typically a MASTER lesson will contain a number of questions, which are included to encourage the student to think about information that may either be deduced or have been presented in an earlier part of the lesson (or package). The wording of such questions usually has a marked effect upon student responses. Vague wording results in generally longer answers, with increased difficulty in analysing the responses. Ideally a question should deal with one central idea and should require only a short

answer. Analysis of the answer may then be performed by choosing the important, expected "keywords".

The reactions of users to wrongly-analysed responses have been observed to be hostile and generally damaging to confidence in the lesson, especially when apparently correct answers are labelled "incorrect". Every effort must be made to cover the widest range of reasonable responses, which invariably means exposing lessons to as much testing as possible before widespread use. Examination of the response files, stored after each MASTER lesson, have often provided alternate answers for questions and occasionally have indicated the existence of problems in the wording of the questions themselves.

Analysing for correctness in response to a question has been found to be straightforward. Similarly responses that are definitely incorrect may be dealt with easily. However there are associated difficulties, largely resulting from inaccurate keywords. The "inexact" matching option, especially, requires considerable attention, as student responses may be incorrectly acknowledged. Answers that are definitely incorrect should generate an explanation of why they were incorrect, wherever possible. In a subject as complex as Chemistry, students may gain an incorrect or incomplete impression of a concept. A carefully considered correction of an answer may therefore have considerable force for a particular student.

Lesson responses to student answers that are either correct or completely incorrect are not difficult. The intermediate level of partially correct answers is however

quite demanding and it is this area of response matching where an Author language may stand or fall. The practice of regarding each non-correct answer as being wrong has little value as a teaching aid. At the very least, a response that does not fall into a recognised category should receive a statement to this effect, although a more meaningful reply is to be preferred. Students seemed willing to accept an admission that a particular response was not understood, especially when presented in the variety of forms included in the teaching package. In contrast, students were often frustrated, in many of the mainframe STAF lessons, by the common phrase "I did not recognise that response", especially when further progress could only be achieved by correctly answering the question.

Student confidence in the teaching package was increased with a number of practices concerning the use of the matching facility. Matching for such answers as "Help", "Dont Know", "No Idea" and null response (entering no answer) should be performed for all but the simplest questions. Depending upon the question, the student might be given further information, a hint at the solution or an explanation of the answer.

Maintaining high levels of confidence in a teaching package is essential to the success of a package as a teaching tool. Responding to student answers that were partially correct, yet lacking an essential element, proved to be a method of maintaining student confidence. By indicating relevant points in a response and expanding upon these points, a seemingly individual reply to a student

answer could be given. On the occasions that these responses were produced student reactions were favourable.

The final part of any question must always be a presentation of the full correct answer. Since the reason for asking a question is usually a desire to review a section of material, students should be given a short, but detailed display of the important, underlying concept.

(3) Analysis of Lessons

The first of the design requirements of the MASTER language was the syntactic analysis of the lesson and subsequent conversion into a form which may be more readily interpreted, in a process analogous to the compilation of programs. As has been indicated, there were three major benefits arising from a separate syntax analysis. Firstly, lesson execution was more efficient and was therefore faster. The second reason was that the physical program size of the interpreter was reduced and the third reason was that errors were less likely to reach the execution stage.

Physically analysing a MASTER lesson was designed to be as simple as possible, with the only requirement being access to the lesson named by the Author. Fatal errors, such as duplication of nodes, incorrect syntax and reference to non-existent nodes, caused the Analyser to terminate with a description of the error. The omission of any reference to a particular node, although possibly indicative of a design fault, was not considered to be a "fatal error" in an otherwise successful analysis. All such nodes were listed at the end of each analysis.

Following a successful analysis three additional files were created on disk, containing (1) data concerning the nodes, (2) the operations and accompanying references to nodes and (3) all of the text, including keyword strings. This last file remained in the form of a "normal" text file and minor changes (in spelling, for example) could be made, enabling the analogous edit-compile-run-edit cycle to be short-circuited.

(4) Graphics

The second deliberately-designed requirement of the MASTER language was that the maintenance of the graphics screen be the responsibility of the Author. It was intended that Authors would be forced to examine and then specify the relationship between the information to be presented and the physical appearance on the screen.

A good textual display may be easily obtained using the various embedded control characters in a MASTER lesson. More complex displays, particularly diagrams, need to be separately constructed by the Author, using the various graphics editors, and may then be accessed by MASTER lessons.

Each display is essentially a complete copy of the graphics screen, stored in a "compressed" form. A graphics screen is a representation of a part of the memory of the computer. Instead of saving a copy of the appropriate portion of memory as a linear series of bytes (taking a tenth of the available disk space) it may be "compressed" by saving it as a series consisting of a counter and a byte, with the counter indicating how many bytes of that

particular type there are (Green, 1983). Since most screen displays have large unused portions (which implies a large number of similar bytes), the "compressed" form offered advantages in both physical storage size (one hundredth of available disk space) and speed of loading. In addition, when a "compressed" display is uncompressed, it need not necessarily replace the current contents of the screen, but may replace, add to or subtract from the screen as required. The Author may therefore overlay diagrams to obtain a variety of effects. For example, in the teaching package, when explaining the general workings of a Continuous Wave NMR spectrometer, the various components were overlayed as required (Chapter VI).

The ability to present prepared screen displays easily proved to be a major asset of the MASTER language. While the use of such external compressed screens is not mandatory it appears that it would be required by most serious applications of the language.

5. SUMMARY

The need for a part of the teaching package to provide Authors with an intelligent interactive capability was recognised after the completion of the simulation programs. The MASTER language was designed to have such a capability, without being overly complicated by a large basic instruction set. The Author is given considerable freedom in designing the text display and facilities are included to to create both simple and complex diagrams, so that the language is relevant to a wide range of applications. For

example, it was possible to write MASTER lessons to introduce and give a background to the various parts of the package, illustrate the important keys on the keyboard, outline the theory in the working of an NMR machine, present questions for reviewing the theory of NMR and discuss the differences between the NMR package and reality (Chapter VI).

The MASTER Language has proved to be successful both as a part of the teaching package and when used by other CAL Authors. Of particular importance has been the relative ease of constructing lessons which contain both reasonable graphics and the ability to interact meaningfully with student users. As with Author languages in general, a major advantage of using MASTER lessons has been the freedom from the detail of programming, allowing the Author to concentrate upon the interaction between student and computer and the design of the screen display.

A key element in the success of the language appears to have been that the role it was to perform was deliberately limited. The MASTER language was designed to present textual information, interact with student users and display essentially static diagrams. It was not intended as a universal CAL language, since the inclusion of all of the features necessary for every CAL application would simply have resulted in the creation of another general-purpose programming language.

Authors may make enhancements to the language directly, by modifying the Analyser and Interpreter. Many of the present features of the language were in fact

included at the suggestion of Authors, as has proved to be common with much courseware development: "...authors very quickly reach the limitations of whatever language they are using. They then clamour for additional capabilities" (Merrill, 1982). It has also proved possible to interface parts of the MASTER Interpreter with a series of animated displays, although at a loss of the generality of the language (Temple, 1986).

CHAPTER VI

THE MASTER LESSONS IN THE TEACHING PACKAGE

As has been indicated (Chapter V), the development of the MASTER language arose from the need for a number of additions to the teaching package. Early in the development of the tutorial programs, for example, there was an obvious need to include questions on the information contained in those programs. Exposing the package to students confirmed the impression that the review of information that could be achieved by including such questions would be useful. In addition the questions satisfied a very apparent expectation held by students, that some sort of test was inevitable.

With each exposure of the teaching package to laboratory classes students highlighted the need for further features through the use of the package, comments to the supervisor or discussion amongst themselves. The two most obvious were the need for some provision for the inexperienced computer-user and the necessity for an introduction to the whole package to allow an informed choice to be made about the various options presented in the initial menu.

After further investigation of student attitudes it was decided to add two new sections to the teaching package; an indication of how the theory of NMR relates to the production of a spectrum and an explanation of some of the differences between the material presented in the package and what students would actually experience. Having

developed the MASTER language, six lessons were constructed to cover the topics of concern: 1) and 2) test questions arising from the two tutorial programs, 3) an introduction to the teaching package, 4) an introduction to the computer, 5) an outline of an NMR machine and 6) the establishment of a connection between the material in the teaching package and that encountered in the laboratory.

1. QUESTIONS ACCOMPANYING THE TUTORIAL PROGRAMS

The major emphasis of the tutorial programs was the clear presentation of theoretical material on Nuclear Magnetic Resonance appropriate to a certain level of undergraduate Chemistry student. The questions associated with each program were designed to be a continuation of this process, rather than a test of knowledge.

As a contrast with the more formal style of the tutorials themselves, the questions were presented in an informal manner. This received a strong positive response from student users.

There were two methods of encouraging student learning used throughout the Questions. In the first, straight-forward questions requiring entry of one- or two-word answers, such as **"The increase in Chemical Shift due to the withdrawal of electron density is called?"**, were used. Where students did not supply a correct answer, a disapproving comment, such as "Since this is quite important, I had hoped that you would have remembered it", was given. By attaching some importance to the answer to a question it was hoped, and indeed confirmed by observation,

that students would review the relevant area of the tutorial programs. The second was used for some of the more complex areas of the theory of NMR. The questions were used as an opportunity to present again much of the information contained in the tutorial programs, but using the difference in style and method of presentation to achieve a new perspective. In this method the questions generally required more understanding and the interactions were generally more complicated. Again the results were encouraging.

Exposure of the package to students of higher ability revealed another use of the questions. A common pattern exhibited by many of those students was to skim through the tutorial programs without necessarily memorising every detail. The questions were then used to review and enhance understanding and, perhaps more significantly, to gauge what areas of the topic were required to be known. These areas were then reviewed where necessary. Students, therefore, exhibited considerable faith in the teaching package, in that the questions were assumed to highlight the key points of the tutorial programs. These observations served to emphasise the importance of careful selection and construction of questions.

(1) Description of the Questions for PART1

Seven questions were included in the Questions associated with PART1. In all cases a maximum of two attempts at any question were allowed, with the help available for the second attempt being dependent on the difficulty of the question.

To illustrate some of the techniques employed in the design of the lessons, two of the questions will be briefly considered.

The question "**What is the nuclear spin for ^{1}H and ^{13}C?**" was the fourth of the lesson and had an expected answer of "Both have a nuclear spin of one half." Entry of the correct answer received confirmation and a note to the effect that a spin of one half implies that the nuclei may take one of two orientations in a magnetic field. A similar review was presented upon the request for help. Most other student responses involved the entry of numbers and received the comment "I think that was probably a guess", which embarrassed many. This comment was effective however since it was generally true and it appeared to increase student confidence in the teaching package. It also prompted students to review the material presented in the tutorial programs.

The seventh question of the lesson was "**The increase in Chemical Shift due to the withdrawal of electron density is called?**" and had an expected answer of "Deshielding". It was, again, intended to clarify a point made in PART1. Students often expressed some confusion about the terminology associated with Chemical Shift, in particular reconciling phrases such as "increase in Chemical Shift" with "decrease in electron density" and "decrease in magnetic field". In the teaching package, few references were made to the field and frequency, while "Chemical Shift" was widely used. The incorrect answer "shielding" was noted and the correct answer given. As with many of the other

questions, a request for help provoked a comment about the importance of the topic followed by the answer, with the aim of encouraging students to review the relevant material.

An additional feature of the questions from both PART1 and PART2 was the inclusion of a score, as requested by students. This score indicated the number of correct answers and was displayed at the completion of the Questions. It seems likely that the inclusion of such a score had a beneficial effect on most students, since the opportunity to compete with the computer appeared to act as a significant incentive to perform well.

(2) Description of the Questions for PART2

While PART1 was designed to make a large amount of information readily available, PART2 placed more emphasis on explanation and illustration, largely because of the increased difficulty of the material. The questions accompanying each program reflected this difference.

Although there were again seven numbered questions, many had several parts and only two were in the simple question-and-answer style of the first set. Instead a style more like the dialogue approach was used, allowing students to take time to concentrate more upon understanding. In addition the questions aimed to extend the theory to more practical topics. This overall approach appeared to be of considerable benefit to students.

Student reaction was generally enthusiastic to these questions, and it was of particular satisfaction to observe students put considerable effort into an answer and for them to receive a similar explanation from the computer. In

order to outline the various techniques employed, full descriptions of all of the questions contained in the lesson are given below.

(a) Question 1. **"What is responsible for the difference of the magnetic field experienced by the nucleus from the applied field?".** The expected answer was "The surrounding electrons."

This question was intended to review some of the material basic to the theory of NMR. Students found the question somewhat different in approach than expected and some were confused about how to continue.

Answers that were not correct received the general hint associated with the question, which suggested that the possible sources of magnetic field around the nucleus be considered. As with many of the questions associated with PART1, the question was asked again with the first answer still visible. The correct answer was displayed after a second attempt or entry of the correct answer.

(b) Question 2. The second question provided the first opportunity for students to apply the facts presented in the tutorial programs.

Two compounds, diethyl ether ($C_2H_5OC_2H_5$) and pentan-2-one ($CH_3COC_3H_7$), were presented in turn. For each compound, students were asked to indicate the fragments which were equivalent.

In the first compound, both methyl groups are equivalent, as are both methylene groups. The second compound has no equivalent groups. For both compounds students were required to enter letters corresponding to the choices of

groups (Figure 6.1). Incorrect choices received an explanation of the reasons.

(c) Question 3. **"Name three important features that neighbouring nuclei must possess if coupling is to occur".** This question invited students to enter as many of the features as they were able. The three major features expected were "Positive nuclear spin", "Must be nearby" and "Must be non-equivalent."

The answer was analysed and the relevant points noted by the computer. If any had not been covered in the answer a request for a further response was made, allowing students to either attempt to complete the entire answer, or to indicate that they were finished. The results of the question were then presented, with the points raised by the student presented and a score out of three given. A presentation was then made of the important features of the question, with the aim of reviewing the material.

(d) Question 4. In question three the subject of the proximity of nuclei involved in Spin-Spin Coupling arose. This was the subject of further investigation in question four. A statement, again reviewing the important points, was presented and indicated that "nearby protons" were responsible for most of the Coupling in ^{1}H and ^{13}C NMR. The question considered the meaning of the word "nearby", and therefore consisted of two parts.

The first part, **"For ^{13}C NMR, where is 'nearby'?"**, had an expected answer of "Directly bonded to the nucleus", while the second, **"For ^{1}H NMR, where is 'nearby'?"**, expected "Attached to the next carbon atom in the molecule."

Students had some difficulty with the first part, usually because the question was more vague than usual and many could not formulate an answer that they thought the computer would understand. Even so there were few cases in which student answers were incorrectly analysed, with the three categories of answer (the answer is known, not known or possibly known) being dealt with successfully. The first two categories received the complete answer and the third a hint.

The second part of the question was more successfully answered, possibly because of practice effects with the first half and possibly because of greater familiarity with ^{1}H NMR.

As with question three, in the summary of the question, emphasis was placed upon the major features of Coupling.

(e) Question 5. **"If there are n protons causing 'splitting' (i.e. non-equivalent and adjacent), into how many peaks will the resonance representing the nucleus be split?"** The answer required was "n+1."

The question proved to be an easy one for students, with almost all entries being either the required answer or an equivalent. When reviewing the material arising from the question, brief comment on the shape of the multiplet was made along with mention of Pascal's triangle.

As with the tutorial programs, there was no mention of situations which were not first order. This was left until the last of the MASTER lessons.

(f) Question 6. A "compressed picture" was used at the beginning of question six to display the idealised ^{1}H and ^{13}C NMR spectra of ethanol (C_2H_5OH), side by side (Figure 6.2). From the information displayed, students were required to decide which was which. Since the resonance arising from the hydroxyl proton was not included in the ^{1}H NMR spectrum, the only information included was the relative positions and couplings of the two multiplets in each spectrum.

Students were first asked which spectrum was which: **"Is Spectrum 'A' the ^{1}H NMR spectrum of Ethanol?"** The expected answer was "Yes." Students were asked to give an answer and were then asked to either review or investigate the reasoning behind the choice, depending on the accuracy of the original answer. The investigation began with a question about the ^{1}H NMR spectrum of the molecule. The question was **"In the ^{1}H NMR spectrum, the quartet represents which group in CH_3CH_2OH?"** Using the "rule" presented in Question 5, the number of neighbouring protons must be three and so the group was deduced to be the methylene (CH_2) group. The computer noted that this group was bonded to the electronegative oxygen atom, and would therefore appear at a higher Chemical Shift than the multiplet for the methyl group (the triplet). Since Spectrum A had the quartet at higher Chemical Shift, it was deduced to be the ^{1}H NMR spectrum of ethanol. A similar outline of why Spectrum B was the ^{13}C NMR spectrum was then presented.

Question 2

Equivalent groups in a molecule have Chemical ELECTRONIC Environments which are identical.

Indicate 2 groups which are equivalent by typing in the TWO appropriate letters (just type NONE if there are none)

1) $CH_3-CH_2-CO-CH_2-CH_3$

A B C D E

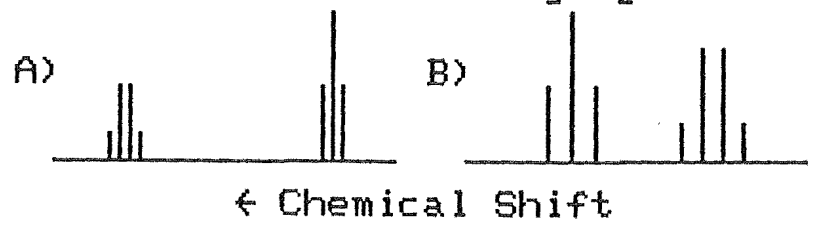
> BD_

Figure 6.1

Determining equivalent protons

Question 6

Study the spectra of CH_3CH_2OH below.



One is the 13C and the other 1H NMR, but which is which ??

Press the RETURN key to continue > _

Figure 6.2

Analysis of the spectrum of ethanol

Student reaction to Question 6 was highly positive. This was largely because the rationales presented by students for the choice of spectra closely resembled those contained in the lesson.

(g) Question 7. The last question of the lesson was **"The method used to determine ratios of protons for peaks in a ^{1}H NMR spectrum is called?"** and had the expected answer "integration." It was a single word fill-in, with the object being to remind students of the relationship between the number of protons and the shape of a ^{1}H NMR spectrum. Students generally answered correctly and rarely needed to take advantage of the unsubtle hint, which referred to the usual method of determining the area under curves.

(3) The Impact of the Questions

There was variation in student reaction to the questions. Key factors influencing this reaction appeared to be the personality and motivation of the student. The most highly motivated generally achieved more from the Questions, in that they were more active participants in the learning process. One of the positive advantages cited by students was the fact that the computer was able to conduct each user at a pace appropriate to that user. In addition, it was felt that the fear of failure was less when questioned by a computer, than by a tutor.

The effect of personality was most clearly exhibited at the completion of each set of questions. Before returning to the teaching package main menu after completing the last question, a score was presented. In both sets of questions it was observed that reaction to the presentation

of a low score was variable, ranging from annoyance (in several cases students repeated the lesson, simply to obtain a higher score), to embarrassment (with an accompanying desire to perform better resulting in a studied review of the tutorial programs), to indifference. Only this last type of reaction was of no longer term benefit to students.

2. INTRODUCTION TO THE TEACHING PACKAGE

After a brief introduction, an approximation of the main menu was displayed, forming the basis for the lesson. Students could easily obtain brief notes upon each of the options, by entering the appropriate letter. When the notes on a particular option had been viewed, the student was returned to the menu to either choose another option or return to the teaching package main menu.

The INTRODUCTION was designed to be a passive tool, to be used to gain information so that an informed choice could be made. The information requested by students was recorded so that improvements could be made to the teaching package main menu, where indicated.

Of all of the MASTER lessons, the INTRODUCTION was the least effective, due both to the style in which it was constructed and to the expectations of the students who used it. These students were generally the less motivated and less able, with most other students willing to make choices based either on the brief synopses displayed in the main menu or to ask for some assistance. The relative lack of success of the INTRODUCTION is a reminder that the merits of

a particular approach in Computer Assisted Learning are determined by the users.

3. INTRODUCTION TO THE COMPUTER KEYBOARD

Throughout the testing of the teaching package, students exhibited a wide range of familiarity with the use of computers. Some were completely familiar with the operation of a keyboard and the jargon associated with computers, while others appeared uneasy at the prospect of using a computer and were bemused by statements such as "Hit <SPACE> to continue", a legacy of early APPLE software. Even after making the instructions throughout the package a great deal clearer ("Press the key marked 'RETURN' to continue"), there was still a need for a lesson to help those students with limited experience.

The major concern of the lesson was therefore to present enough information to users, so that the various parts of the teaching package could be used. It was decided to illustrate the function and physical position of the important keys on the keyboard as clearly as possible. With this in mind a representation of the keyboard was displayed on the screen, illustrating the positions of the keys. Description of the importance of the various keys then took place. As each key was discussed, its position was highlighted in the display.

The KEYBOARD lesson was generally effective for those who used it, largely due to two features. The first was that its purpose was clearly and simply indicated in the teaching package menu, which meant that only students who

needed to use it did so. The second was that students were conducted through the various descriptions and exercises.

4. THE NMR MACHINE LESSON

A lesson on the theory of the workings of an NMR spectrometer was included to illustrate the connection between the theory presented in the tutorial programs and the practice of obtaining an NMR spectrum from a compound. In keeping with the level of information presented, the explanation was simplified, with the outline of a Continuous Wave spectrometer being used as an illustration, rather than the more complicated Fourier Transform system.

While the preparation of a simple summary of the function of the machine was straightforward, the schematic representations included in many text books (for example, Becker, 1980, p.44, Bovey, 1969, p.5 and Williams and Fleming, 1966, p.79) appeared to be too complicated for easy assimilation. This problem was alleviated by constructing a series of diagrams corresponding to the various parts of the machine and overlaying them in a coherent series, culminating in a complete diagram.

(1) Detail of the lesson

The lesson was intended to complement the first of the two tutorial programs and to be utilised after the material in that program had been viewed. Students using the lesson were therefore asked if PART1 had been viewed. If they had not, the advice was given that that course should be considered and if so desired the lesson could be terminated.

Students could however proceed and receive a summary of the relevant theory. At various stages of the summary, students were asked about their level of comprehension. If students felt that it was inadequate the lesson could be terminated and the tutorial programs started. Students who had previously viewed the tutorial programs were also asked if a review of the theory was required. If it was, the same summary was presented.

A simple diagram of a Continuous Wave Spectrometer was then constructed by overlaying its various components. Firstly the fixed magnet was displayed followed by the "transmitter" coils (Figure 6.3), which provide energy for the change in energy levels. The "sweep" coils, which vary the magnetic field, were then displayed, followed by the "receiver" coils, which receive the retransmitted signal from the nuclei that have been "flipped". Lastly the sample was added, completing the diagram (Figure 6.4).

The final part of the lesson was a short comment advising students who has earlier indicated that they had not seen the tutorial programs that they should do so next.

(2) The Impact of the NMR Machine Lesson

Students were receptive to the lesson. Indeed there were no adverse comments and few questions about the material, and a general satisfaction with the presentation was expressed.

There can be little doubt that the success of the lesson was largely due to the simplicity and clarity of its presentation. In addition the lesson was complementary to the usual sources of student information, since its approach

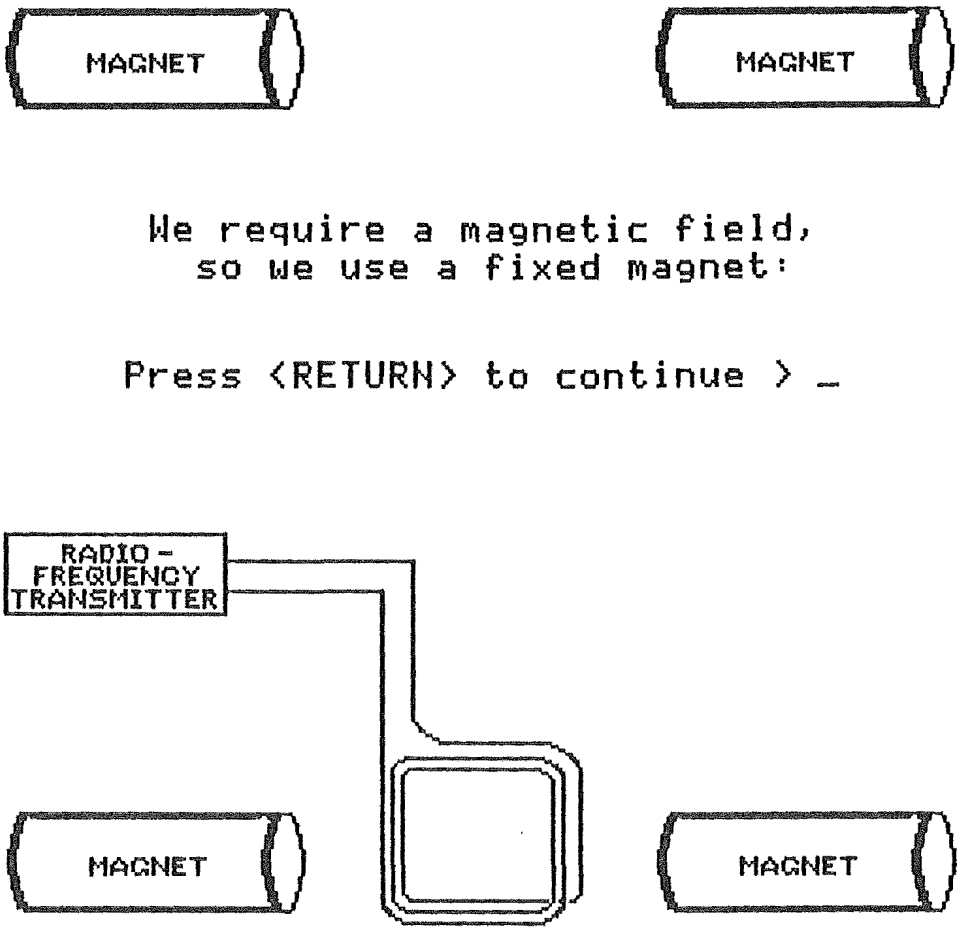
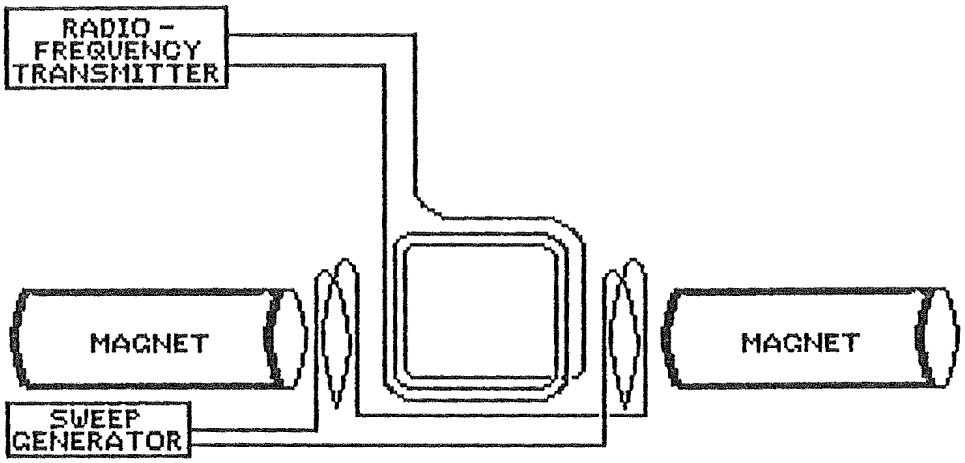


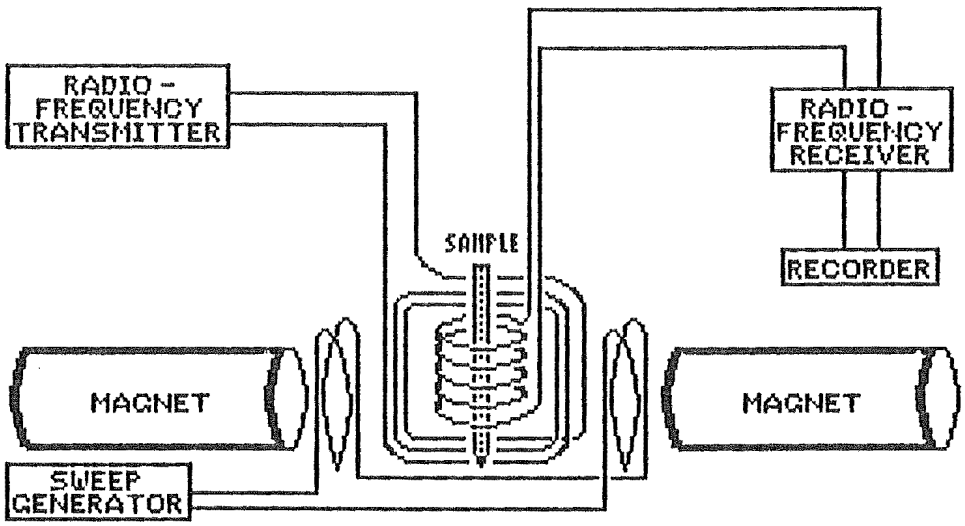
Figure 6.3

Two screen images showing the overlaying used to illustrate a Continuous Wave spectrometer



... and so we use 'sweep coils'
which are placed perpendicular
to the transmitter coils.

Press <RETURN> to continue > _



I hope this helps in your
understanding of the theory of NMR.

Press <RETURN> to continue

Figure 6.4

Screen images showing overlaying in the NMR Machine lesson

was similar to many of the textbooks commonly used.

The underlying method embodied in the lesson is also applicable to most other areas of Chemistry likely to be the subject of computer teaching packages.

5. THE TUTORIAL LESSON

There were two major reasons for the creation of the sixth of the MASTER lessons. Throughout the teaching package a number of approximations had been made (such as the representation of spectra) and a number of details omitted (coupling constants for example), to minimise the amount of material presented to students. It was therefore considered desirable to outline some of these details in a part of the package. The second reason for constructing the lesson was the desire that students be able to relate the material presented directly to laboratory work. By outlining the approximations and omissions it was felt that these aims could be achieved.

(1) Content of the Tutorial Lesson

The TUTORIAL lesson was designed in four parts, the first three of which were essentially new topics: notes on the differences between the appearance of spectra in the teaching package and the laboratory, the appearance of an actual ^{13}C NMR spectrum, and Coupling Constants. The last part was a survey of an application of NMR and included many of the important features raised throughout the teaching package. Unlike most of the other lessons in the package, it was intended that the various parts of the TUTORIAL

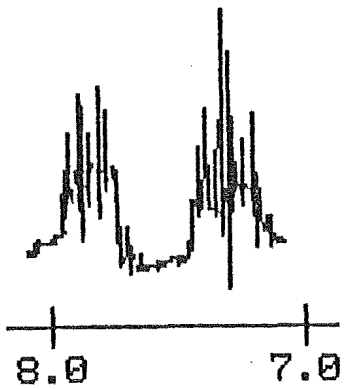
lesson be accessible independently, even though, as predicted, most students did not make use of this ability.

(a) The First Section. The first section of the TUTORIAL lesson noted that the spectra displayed throughout the teaching package were idealised when represented as groups of vertical lines. Mention was made of the possibilities of peak broadening, non-appearance of resonances and the complexity of some resonances. The ^1H NMR spectrum of propiophenone ($C_6H_5COC_2H_5$) was used as an example of the latter (Figure 6.5).

(b) The Second Section. The second part of the lesson concentrated upon Coupling Constants. By introducing the subject gradually and engaging in some dialogue with students, it was felt that new information could be presented in a satisfactory manner. Students did in fact appear receptive to this information.

One of the compounds from the analysis program, 1-nitropropane ($C_3H_7NO_2$), was used to introduce the topic, by investigating the sextet in its ^1H NMR spectrum. To explain the source of this sextet the effects of the two neighbouring groups (a CH_3 and a CH_2) were displayed.

Overlays were used to construct complex diagrams, by changing relatively small parts of the screen. This allowed students to study the effect of the methyl group (Figure 6.6), the coupling constant and the addition of the methylene group (Figure 6.7). The effect of a methylene group in a compound where the Coupling Constants were not essentially equivalent was then investigated (Figure 6.8).



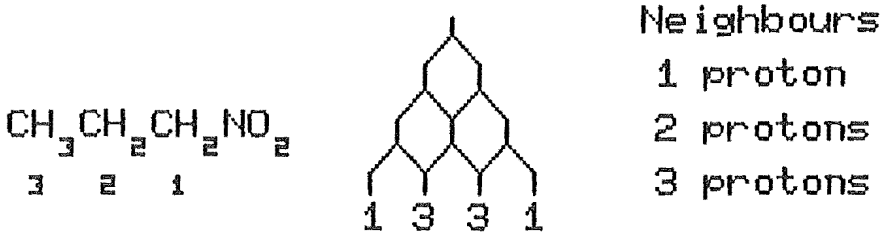
For example in the ^{1}H NMR spectrum of propiophenone ( $COCH_2CH_3$),

there is a complex multiplet where we expect benzene resonances.

Press <RETURN> to continue > _

Figure 6.5

Part of the proton spectrum of propiophenone

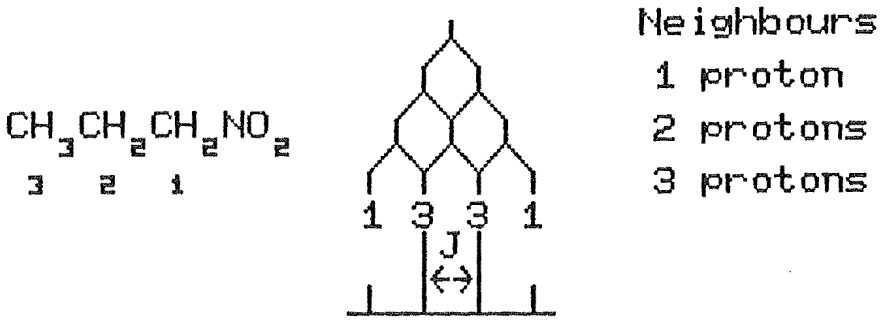


As you might expect we find that the result is a quartet.

Note that the intensity of each peak can be deduced from Pascal's triangle or from the number of different pathways to each end in the above diagram.
Press <RETURN> to continue > _

Figure 6.6

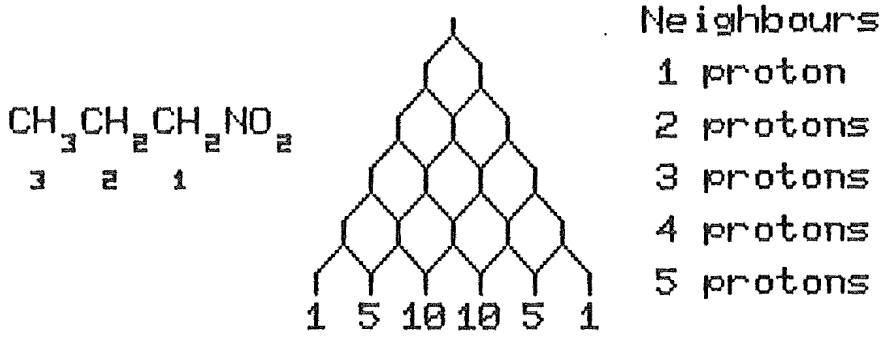
Coupling of a methylene group due to the effect of a neighbouring methyl group



We call the peak separation,
in Hertz, the COUPLING constant, J.

The coupling constant between
the CH_3 and the middle CH_2 is J_{23}

Press <RETURN> to continue > _



Now to add the effect of the CH_2
we must take account of its J value
{ J_{12} for this interaction }.

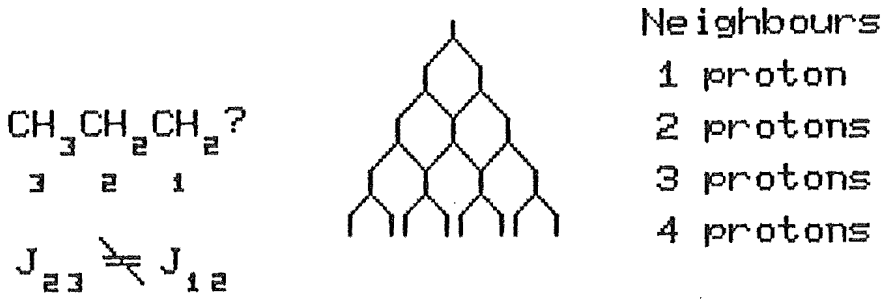
In $CH_3CH_2CH_2NO_2$ it has almost
the same as the J_{23} value.

Press <RETURN> to continue > _

Figure 6.7

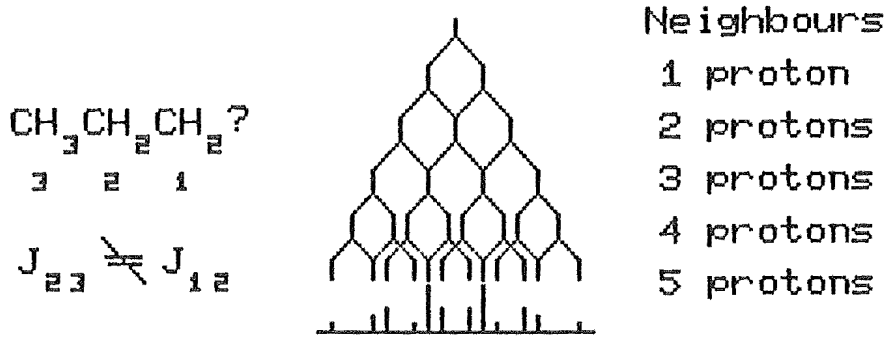
Two screen images showing the effect of

equivalent Coupling Constants



Let's add 1 of the two protons of a CH_2 group with a different J value to J_{23}.

Press <RETURN> to continue > _



The result would look
something like the multiplet above,

with ratios 1:2:3:1:6:3:3:6:1:3:2:1.
Press <RETURN> to continue > _

Figure 6.8

Two screen images showing the effects of

non-equivalent Coupling Constants

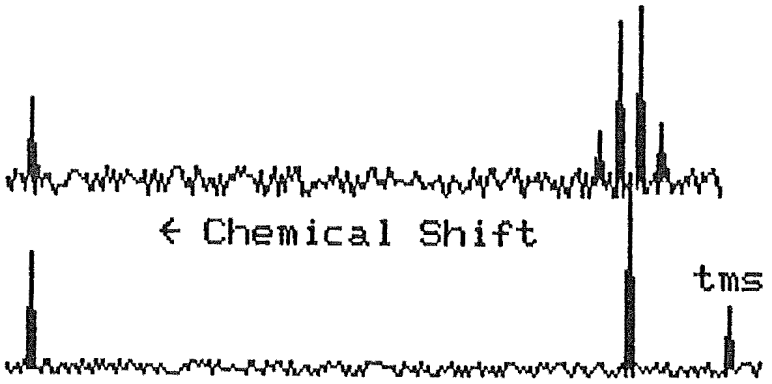
(c) The Third Section. The third section was included to prepare students for the actual ^{13}C NMR spectra that they would receive in laboratory sessions.

The first display (Figure 6.9) consisted of two displaced ^{13}C NMR spectra of acetone (CH_3COCH_3), in the form commonly encountered in laboratory classes: the bottom spectrum being spin-decoupled. Having indicated the differences between the two spectra, the advantages of the decoupled spectrum were outlined (Figure 6.10).

Students were encouraged to identify the compound, using the information deduced from the spectra. The quartet arising in the resonance at lower Chemical Shift led to the deduction of a methyl group (CH_3), while the resonance at higher shift suggested a carbonyl group (CO). Although few students arrived at the correct answer without assistance, none experienced any apparent problems with the dialogue and all showed a ready acceptance of ^{13}C NMR spectroscopy.

(d) The Fourth Section. The final section of the TUTORIAL lesson was included more as an example of NMR in use, than an attempt to present new information. A representation of the ^{1}H NMR spectrum of ethylvinylether ($C_2H_5OCH{:}CH_2$) was displayed (Figure 6.11) and then analysed in detail (Figure 6.12).

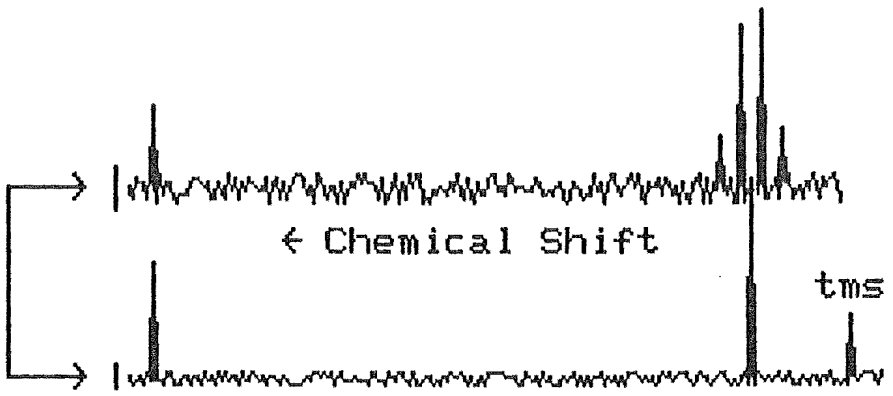
The terms "cis", "trans" and "gem" were discussed and the magnitudes of the various Coupling Constants between the three protons associated with the double bond noted (Figure 6.13). As with the previous part of the lesson, levels of student concentration and understanding seemed to indicate that the manner of presentation of the material was



The next section is another interesting
aspect of NMR in greater detail...
CARBON-13 NMR.

Figure 6.9

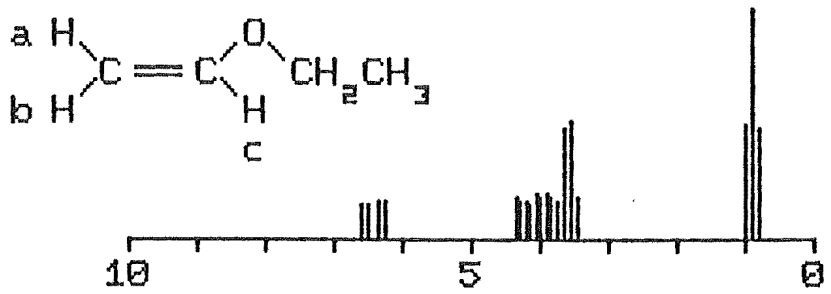
^{13}C NMR spectrum of acetone



The bottom spectrum is SPIN-DECOUPLED
which makes it less confusing
(a singlet for every type of carbon)
and improves the signal-to-noise ratio.
Press <RETURN> to continue > _

Figure 6.10

Differences between coupled and decoupled ^{13}C NMR spectra



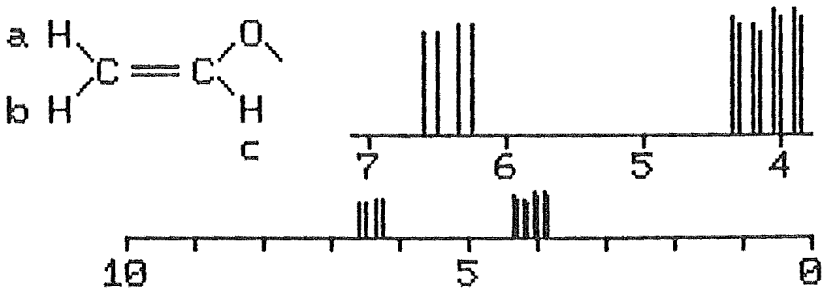
Coupling in Olefins

Here is the proton NMR spectrum of an organic compound with a double bond (ethylvinylether).

Press <RETURN> to continue > _

Figure 6.11

^{1}H NMR spectrum of ethylvinyl ether



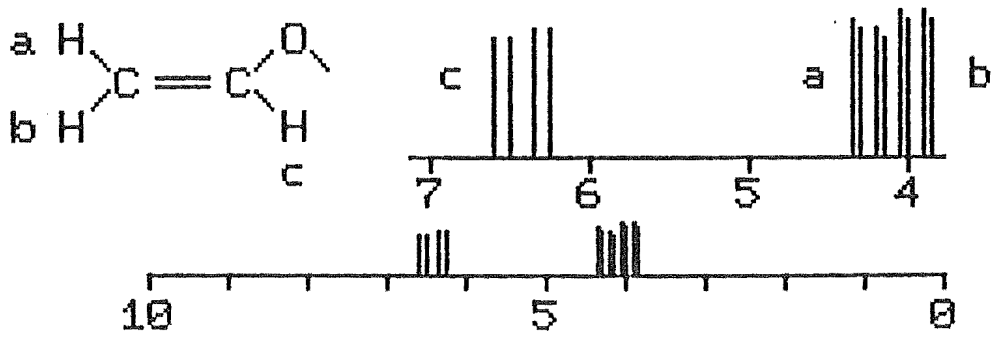
The remaining parts of the spectrum are a little hard to see, so I'll expand the scale a bit.

Note that the peaks are still idealised.

Press <RETURN> to continue > _

Figure 6.12

Analysis of the spectrum



The coupling constants are, by size:
$J_{gem} < J_{cis} < J_{trans}$

where gem, cis and trans refer to the relative positions of the PROTONS
(ie $J_{gem} = J_{ab}$)
So therefore $J_{ac} > J_{bc} > J_{ab}$

Press <RETURN> to continue > _

Figure 6.13

Coupling constants in the spectrum

appropriate for student comprehension.

The lesson finished with a reference to a suitable text book (Abraham and Loftus, 1978) for further study.

6. SUMMARY

The advent of the MASTER language and the inclusion of the MASTER lessons in the teaching package proved to be important in its development. The ability to present material of a common general form easily proved to be of considerable value, since much of the detail associated with any programming task was removed. The six lessons were received by students with varying degrees of enthusiasm, but all, with the possible exception of the INTRODUCTION, were successful in both intent and execution.

CHAPTER VII

ASSESSING THE NMR TEACHING PACKAGE

An important part of the development of the package was an assessment of its effectiveness. Discussions with professional educationalists at Canterbury University led to the conclusion that an such assessment would need to consist of two distinct parts: an evaluation of student attitude towards the teaching package (and related areas) and an evaluation of the effectiveness of the package as a teaching tool.

1. ADMINISTRATION CONDITIONS

The students selected for exposure to the teaching package were in a group of approximately half of all of those at the Stage 2 level involved in Organic Chemistry laboratories. At this level the laboratories were held as two separate sessions, with about half of the students in each. There were two types of student involved in the laboratories. The majority were involved in a three-year course to obtain a Bachelor of Science degree and their abilities and experiences covered a wide range. A smaller number were part of the more advanced four-year Bachelor of Science with Honours course and all possessed higher-than-average abilities.

It is in these laboratories that students receive most exposure to the subject of NMR. Students were often

introduced to a variety of apparatus in the laboratories and the appearance of the computer was therefore not unusual. One computer was available for six weeks for all eight hours of each laboratory session, with additional use possible upon request. In line with normal practice, the use of the computer was to have been on a voluntary basis, the intention being that students would make use of it in the lulls between experimental work. However so little time was spent on the computer under this arrangement that its use was made compulsory. This was in conflict both with the underlying philosophy of the teaching package and with the pattern of exposure to earlier groups of students.

Both scales were administered in the last laboratory session of the year. The Attitude scale was administered to all of the B.Sc. students and to the Honours students of comparable level.

Administration of the Achievement scale posed some problems. In an ideal situation, two groups of B.Sc. students would have been compared, one having had exposure to the teaching package and the other one not. However this would have required comparison of students in different laboratory sessions and would have meant that one group would have been alerted to the "test", with a possible effect on performance. The construction of a parallel test would have been an additional necessity. Instead the less satisfactory alternative of comparing those B.Sc. users of the teaching package against the Honours class with a laboratory session on the same day (and any B.Sc. students who had not used the computer) was chosen.

2. THE ATTITUDE SCALE

The general aims behind the Attitude scale were, for those having used the teaching package, to determine whether it was effective, easy to use, worth applying to other Chemistry topics and how it compared with other teaching methods. For those not having used the computer an assessment of student expectations of and possible reception to CAL material was planned.

It was initially envisaged that the scale would have three sections (the teaching package, CAL in Chemistry and NMR as a Chemistry topic) and that it would be administered to everybody. However it became obvious that two separate, but overlapping, scales would be more effective. The scales would be for users and non-users.

It was decided to construct a Likert scale, since that style was in common usage at the University and it would have been previously encountered by many students. Technical information for the construction of the scales was obtained from a number of sources (Anastasi, 1976, Oppenheim, 1966, and Shaw and Wright, 1967).

In a Likert scale the student is asked to respond to a series of statements in one of five ways: Strongly Agree (SA), Agree (A), Neutral (N), Disagree (D) and Strongly Disagree (SD). Evaluating the response involves assigning a value to the option the student has chosen. For example if agreement with the statement is deemed to be a positive attitude SA is assigned the value 5, A the value 4, N 3, D 2 and SD 1. If a statement is negative the values are reversed.

The items in the scale may therefore be analysed individually, by considering mean and standard deviation, and as a part of the whole scale by considering the correlations of the item scores with the total score and other item scores. Item scores can be added to give a total attitude value for the student, provided that all of the items in the scale correlate reasonably with the total score. A scale which has all of its items measuring the same basic attitude is said to be unidimensional. An outline of some statistical methods is given in Lindeman and Merenda (1979).

(1) Attitude Scale for Teaching Package Users

The users' scale consisted of 20 items, numbered as presented to students. A list of these items with positive or negative character indicated is given in Table 7.1.

Having been assigned values, the students responses were analysed and the mean and standard deviation values, inter-item and total score correlations were obtained for each item.

(a) Elimination of unsuitable Items. In order to perform a thorough analysis, an Attitude scale needs to be unidimensional. The preliminary results indicated that this was not the case and that certain items, as indicated in Table 7.1, needed to be eliminated.

Items 6 and 16 were both concerned with the comparison of the teaching package and laboratory demonstrators. The items had moderate correlations with the total score, but no significant inter-item correlations except with each other (0.719). This at least indicated that a consistent response

Table 7.1

The Users' Attitude Scale

1. I found the computer exercise helpful.
2. The time spent on the computer was worthwhile.
3. The exercise would have been useful to almost all of the class.
4. Similar exercises would be useful for other Chemistry topics.
5. The computer exercise was of limited value for the time spent on it.
6. The time spent on the computer would have been better spent with a demonstrator.
7. A text book would have been just as good as the computer.
8. The CAL exercise is a valuable learning aid.
9. The computer was probably the best method of teaching NMR.
10. I found the computer difficult to use.
11. I could get at least as good an understanding of NMR in the library as I could get from the computer exercise.
12. Overall the computer exercise was impressive.
13. I thought that using the computer was straightforward.
14. The computer exercise was, in total, excellent.
15. The computer exercise appeared to cover the topic of NMR well.
16. I think a demonstrator could help me as much as the computer exercise could.
17. I hope that more Computer Assisted Learning (CAL) material is made available in future.
18. Compared to other methods of teaching (lectures, textbooks and demonstrators), CAL is too limited to be really effective.
19. Chemistry lecturers should utilise Computer Assisted Learning to complement lecture courses.
20. The place of CAL is in augmenting laboratory work.

Alignment of Items in the Users Scale

Positive Statements 1 2 3 4 8 9 12 13 14 15 17 19

Negative Statements 5 6 7 10 11 16 18 20

Items for Elimination

Item	Mean	Standard Deviation	Correlation with total score
6	3.3333	0.8357	0.3965
16	2.9524	0.8985	0.3766
10	3.9048	0.9209	0.3957
13	4.0000	0.6901	0.3124
11	3.3810	0.7854	0.3181
15	3.9048	0.4259	0.3699
20	2.7619	0.6835	-0.1280

was provoked. These items are, however, measuring another factor apart from the desired one, possibly an "attitude to demonstrators" factor. Comments written by students further reinforced this belief.

Correlations of items 10 and 13 with the total score and with most other items are at best moderate, although the two correlate highly (0.749) with each other. While indicating that the use of the teaching package was not considered difficult by students, the items were excluded from the analysis of the scale since they offered little of value to it.

In its wording item 11 was superficially similar to item 7 (mean 3.4762, standard deviation 1.0057 and correlation with total 0.6184). The intention in both of these items was that the teaching package should be compared with a text book. However the correlation of the two items (0.554) is much lower than that between other pairs of similar items (as above, items 10 and 13 at 0.749 and items 6 and 16 at 0.719). While item 11 had some moderate correlations with other items, it seemed likely that there were connotations associated with the mention of the "library" which resulted in its exclusion.

Item 15 was originally included in order to test whether there were any apparent inconsistencies or deficiencies in the teaching package. The item had a favourable and uniform response, which probably indicated that the package covered everything that students had been exposed to. However as with items 10 and 13, the item offered little to the scale and it was similarly excluded.

That there were problems with item 20 was obvious from the comments of students as they completed the scale, generally indicating that the meaning of the statement was not entirely clear. There was additional difficulty in determining whether the statement was a positive or negative one. The negative correlation with the total score suggests that the eventual choice was incorrect. The mean and standard deviation values indicate that most students opted for the neutral response. The only benefit arising from the item was that it elicited some comments from students, which generally indicated that the computer should be used in, but not confined to, the laboratory.

(b) Data for the Final Attitude Scale. After eliminating the unsuitable items, the remaining thirteen fell roughly into four categories: 1) the value of the teaching package (items 1, 2, 3, 8 and 5), 2) the place of the package and its comparison with other standard teaching methods (7, 9, 19 and 18), 3) the overall impression of the package (12 and 14) and 4) the possible reception to more CAL material (4 and 17). Many of the items do, however, overlap into more than one category. The data for these items were re-analysed and appear in Table 7.2.

In this Table, the "item-total score" correlations were made between item score and total score minus item score, to allow for the contribution of the item score to the total. This allowed the significance of the correlations to be calculated: correlations greater than 0.4329 were significant at the 0.05 level (a probability of less than 0.05 of the numbers arising by chance) and greater

Table 7.2

Data for the Users' Attitude Scale

Item	Mean	Standard Deviation	Correlation with total score
1	4.1905	0.6633	0.5852
2	3.8095	0.7315	0.7899
3	3.7143	0.6281	0.6181
8	4.0952	0.6098	0.6768
5	3.3810	0.7854	0.4854
7	3.4762	1.0057	0.6458
9	3.0476	0.6529	0.8078
19	3.6667	0.9920	0.4567
18	3.5238	1.0057	0.4494
12	3.7619	0.6835	0.6856
14	3.5714	0.8492	0.7982
4	4.3810	0.4856	0.6324
17	4.1905	0.5871	0.4159

The Total Score had a mean of 48.810 and a standard deviation of 6.6089.

Significant Inter-Item Correlations

(All values multiplied by 1000)

	1	2	3	8	5	7	9	19	18	12	14	4
2	664											
3	772	503										
8	544	574	693									
5	-	624	-	-								
7	-	576	-	547	434							
9	-	617	614	587	-	618						
19	-	-	-	-	-	589	539					
18	564	589	-	-	-	-	-	-				
14	520	481	618	511	435	-	666	-	-			
12	652	712	485	539	-	462	638	452	709	645		
4	-	472	-	-	743	604	544	-	-	-	-	
17	-	-	-	-	-	-	597	-	-	588	-	581

than 0.5487 were significant at the 0.01 level.

Although the correlations between item and total score and between item and item were calculated (Table 7.2), a factor analysis of the data was not undertaken. Factor analyses are typically performed in detailed attitude studies and consist of further refinement of the data to determine the small numbers of factors that are being measured by the attitude scale (Anastasi, 1976). Since the quantitative analysis detailed above was considered adequate for this study, a factor analysis was not performed.

(c) Meaning of the User Attitude Scale. When taken together, items 1, 2, 3, 5 and 8 indicate that students thought that the teaching package was both helpful and worth the time spent on it. Interestingly, item 5 has a much lower mean value than the other four items, even item 2, the other "value for time spent" statement. Since items 2 and 5 correlated significantly, there must have been another effect to account for in the response to the latter. This effect was probably the high expectation of the performance of a computer in a teaching session. Analysis of the non-user attitude scale and observation of student behaviour supported this conclusion.

Of the four items included in the second category, three: 7, 9 and 19, intercorrelated significantly. The responses to item 7 indicate that students, on average, found the teaching package to be moderately preferable to a text book for learning. Opinion was neutral as to whether the computer was the best method of teaching NMR (item 9), with the students with a more favourable overall attitude

being most in favour. Item 9 was an example of the effect of the intensity of statement wording upon response. Students were moderately in favour of the teaching package being used in conjunction with lecture courses (item 19). Item 18 was included in this category as it appeared to cover the same approximate area as the other three items. Although there were some adverse comments, generally students indicated that the limitations of CAL were not apparent.

Students were generally favourably impressed with the teaching package judging by the responses to items 12 and 14. These items were very similar and the slightly different responses are a result of differing statement intensity.

That there was a strong desire for more, widely-available CAL material was indicated by the definite responses to items 4 and 17. Comments on the need for similar exercises were also common.

(2) Attitude Scale for Non-Users

The Non-Users' scale consisted of nine items. A list of the items and their positive or negative rating is given in Table 7.3.

Having been assigned values, the student responses were analysed and the mean and standard deviation values as well as the inter-item and total score correlations were obtained for each item. Descriptions of the methods used in the various analyses appear in Lindeman and Merenda (1979).

Table 7.3

The Non-User's Attitude Scale

1. Computer Assisted Learning (CAL) is a valuable part of Chemistry.
2. There isn't much scope for CAL in Chemistry.
3. I hope that CAL material becomes widely available in future.
4. Computer Teaching material will never be of major importance in Chemistry.
5. Compared to the other methods of teaching (lectures, textbooks and demonstrators), CAL is too limited to be really effective.
6. Chemistry lecturers should utilise Computer Assisted Learning to complement lecture courses.
7. The place of CAL is in augmenting laboratory work.
8. I would not use a computer in preference to any other method of learning.
9. I can't see how a computer could really help me learn Chemistry.

Alignment of Items in the Non-User Scale

Positive Statements	1 3 6
Negative Statements	2 4 5 7 8 9

Items for Elimination

Item	Mean	Standard Deviation	Correlation with total score
5	3.5000	0.8507	0.2647
7	2.8947	0.7877	0.0031

(a) Elimination of unsuitable Items. Examination of the preliminary results indicated that two of the items (5 and 7) needed to be deleted in order to preserve unidimensionality (Table 7.3). Item 5 had a low correlation with the total score and only one significant correlation with other items. This item required students to give an opinion on a subject which they may not have had exposure to. It was therefore not reasonable to retain the item. Item 7, as in the Attitude scale for users of the teaching package (where it was item 20), was deleted from the final scale for similar reasons. Written student comments accompanying the item were generally similar also, with several noting that augmenting laboratory work was not the only role the computer should take.

(b) Data for the Final Attitude Scale. The seven items in the final scale had moderate to high correlations. The final results are summarised in Table 7.4, where correlations greater than 0.3206 are significant at the 0.05 level and greater than 0.4132 significant at the 0.01 level.

As with the User Scale, the correlations between item and total scores were adjusted to allow the significance to be calculated correctly and a factor analysis was not required.

(c) Meaning of the Non-User Attitude Scale. Students thought that Computer Assisted Learning was an important and valuable part of Chemistry and hoped for CAL material to become more widely-available in the future (items 1, 2, 3 and 4).

The high expectations of CAL material were indicated by the responses to item 9, but that there was a realistic attitude prevalent was shown by the responses to item 8. When the result for this latter item was taken in conjunction with that for item 6 in particular and the others in general, there is an implication that students saw CAL as being a valuable part of the Chemical Education system, especially as a complement to traditional lectures.

(3) Reliability and Validity of the Attitude Scales

The demonstration of reasonable values for the reliability and validity of a scale is an important indicator of the applicability of its results (Anastasi, 1976). The final form of the attitude scales resulted from a desire to maximise these values.

"Split-Halves" Reliabilities, with the Spearman-Brown correction for scale length, were calculated for each scale, giving the highly satisfactory values of 0.869 for the User scale and 0.810 for the Non-User scale. In addition the fact that the scales had reasonably high reliabilities can also be illustrated by considering the responses to similar items as noted above. This fact indicated a level of consistency in each of the scales.

Further indication of this was given by the fact that the four items that were included in both scales provoked essentially the same responses (Table 7.5). In Table 7.5, the first item in each pair was presented in the Non-User Attitude scale, while the second was presented in the User Attitude scale.

Table 7.4

Data for the Non-User's Attitude Scale

Item	Mean	Standard Deviation	Correlation with total score
1	3.8158	0.8539	0.6611
2	4.0789	0.8998	0.4804
3	4.2368	0.6255	0.7043
4	4.1053	0.8204	0.5098
6	3.7895	0.7312	0.5345
8	3.0526	0.9719	0.4203
9	4.2632	0.4403	0.4404

The Total Score had a mean of 27.342 and a standard deviation of 3.6366.

Significant Inter-Item Correlations

(All values multiplied by 1000)

	1	2	3	4	6	8
2	361					
3	772	528				
4	478	-	413			
6	444	465	397	344		
8	424	-	326	356	-	
9	-	346	442	-	336	337

Table 7.5

Comparison of Items in the Attitude Scales

Item	Mean	Standard Deviation	Correlation with total score
3	4.2368	0.6255	0.4140
17	4.1905	0.5871	0.4340
5	3.5000	0.8507	0.2647
18	3.5238	1.0057	0.4628
6	3.7895	0.7312	0.4659
19	3.6667	0.9920	0.4654
7	2.8947	0.7877	-0.0031
20	2.7619	0.6835	-0.1280

Each of the last pair of items was also accompanied by similar written comments, as students attempted to clarify what they meant by their responses.

A high Construct Validity was ensured by retaining only those items which exhibited a high correlation with the total attitude score and with the other items in the scale.

(4) An Overall Summary of Student Attitudes

Students had a favourable attitude towards Computer Assisted Learning in Chemistry, both in general and to the teaching package. Cavin et al. (1980) noted a similar tendency in student attitude. Widespread opinion held that CAL material should be more accessible and should cover more subject areas: suggestions being as varied as benzene chemistry, reaction mechanisms, electron orbital splitting and ligand reactions.

As far as defining a role for the computer in Chemical Education, students agreed with the suggestions for augmenting traditional lectures. Written comments reinforced this point, indicating that the computer is perhaps best at reviewing and expanding upon material that the student user has already encountered. As one student commented, the computer was good for "teaching rather than lecturing." Similar opinions were expressed in Offir (1983).

Some students who had not used the computer commented on the possible limitations of CAL in coping with students of differing abilities. However the prevalent attitude was that such limitations were not evident and there were many

comments welcoming the freedom to learn at a comfortable and unpressured pace using a computer.

In total the attitudes of students indicate that the NMR teaching package conformed to the high student expectations of successful Computer Assisted Learning.

3. THE ACHIEVEMENT SCALE

The purpose of an achievement scale, henceforth referred to as the "test", was to gauge student knowledge of NMR and to assess any differences exposure to the teaching package might have caused. Of particular interest were the relative levels of rote-learning (memory), actual understanding, and ability to apply knowledge displayed by students.

The test was to be criterion-referenced, in that it was designed to assess mastery of the subject rather than performance relative to other students (Popham, 1978). It will be seen, however, that the overall level of mastery was somewhat lower than expected.

As has been indicated previously, there were constraints on the amount of exposure students had to the teaching package. This, coupled with the fact that its use needed to be made compulsory, implied that students were generally less motivated for the learning experience than previous groups.

(1) Content of the Achievement Scale

Before the test was constructed, the various parts of NMR necessary for inclusion were determined, using three

principle sources. These were the laboratory manual, which contained an outline of and exercises on NMR, lecture material and the commonly-used text books. Examination of this material suggested that the test cover three general areas. The first of these was the background theory of NMR, including the concepts of nuclear spin, chemical shift and spin-spin coupling, the gyromagnetic ratio and the various equations. The second was the appreciation of the actual Chemical Shifts, especially the relative values of the more commonly occurring fragments of compounds. The third was the ability to analyse and predict spectra.

The test was constructed in three sections, corresponding to the three general areas (Appendix C). The first section consisted of ten questions about the background theory. The second section was an examination of Chemical Shifts of common fragments and the third was an analysis of ^{1}H and ^{13}C NMR spectra. A number of references were used in the construction of the test (Anastasi, 1976, Cockburn and Ross, 1977, Cronbach, 1961, Heywood, 1977, Popham, 1978, Rowntree, 1977 and Tittle and Miller, 1976).

(a) Section One of the Test. A review of two of the "test" questions is included as an illustration of the content of the section.

The third question asked students to "Give the values for the nuclear spin for the following nuclei: ^{13}C, ^{1}H, ^{15}N, ^{12}C, ^{16}O." All nuclei except for ^{15}N were commonly associated with NMR teaching courses. This was reflected in the results, where no students gave the correct answer of 1/2 for ^{15}N. The other nuclei (with values of 1/2, 1/2, 0 and 0

respectively) constituted a reasonable measure of the depth of student knowledge, having a good discrimination between the higher and lower students.

The sixth question had three parts, each requiring "true" or "false" answers. Chemical Shift was the subject of this question and the various parts asked whether the "relative chemical shift" depended on: "the magnetic field applied to the nucleus", "the nucleus itself" and "the electronic environment of the nucleus." The question was a moderately good one, with the first two parts showing reasonable discrimination values (0.42 and 0.50). The required answers were "false", "true" and "true" respectively.

(b) Section Two of the Test. The second section of the test was concerned with testing student appreciation of Chemical Shift. Students were asked to plot, on a continuum, the approximate Chemical Shifts of a variety of common fragments.

(c) Section Three of the Test. Assessing the ability of students to apply their knowledge and to test and develop skills was the object of the third section of the test, which was further divided into three parts. The first part involved the deduction of a compound, given its ^{13}C and ^{1}H NMR spectra. The compound was propiophenone (ethyl benzyl ketone, $C_6H_5COC_2H_5$). Part two required students to predict the ^{1}H NMR spectrum of methyl-4-keto-hexanonate ($CH_3CH_2COCH_2CH_2COOCH_3$), while the ^{13}C NMR spectrum of butylvinyl ether ($C_4H_9OCH{=}CH_2$) was requested in part three.

(2) Administration of the Achievement Scale

The test was administered to students on the final day of Organic Chemistry laboratories for the year. There were some differences in the manner of presentation of the test to the two groups of students: the users of the teaching package and the non-users. The differences in administration of the "test" were a result of its integration into a laboratory class, with the tutors controlling each class interpreting their instructions differently. There was no deliberate difference in each administration.

The Honours students (non-users) had three quarters of an hour advance warning of the test, but were told that it would not count towards either their final grade for the Organic Chemistry paper, or their laboratory grade. This time was apparently spent upon normal laboratory activities and not upon studying the topic of NMR. The students spent half an hour on the test, which allowed them to complete as much as they were able. In contrast the students in the "users' group" had no warning, were not told that the test would not contribute to their grades (although most guessed correctly that it would not). Students completed the test over the period of about an hour, the longer period being due to a concurrent experiment. In both instances, students were allowed to complete as much of the test as possible without time pressure.

(3) Reliability and Validity of the "Test"

As has been noted previously, the assessment of the reliability and validity of a test is important. Accurate assessment of the reliability of an achievement test is

often difficult, especially when the test is only administered on one occasion. While one measure of internal consistency applied to section 1 of the test (the Kuder-Richardson Formula 20 Correlation Coefficient) yielded a moderate value (0.411), most effort concentrated upon an assessment of the validity of the test.

The validity of a criterion-referenced test is usually assessed by a careful examination of its component parts. The Achievement Scale appeared to have an extensive and properly-weighted coverage of the subject material.

Four types of validity were assessed for the test. Reasonable Content Validity was ensured with extensive planning of test coverage and an examination of the various parts and associated weightings indicate a moderate Face Validity. Since all of the sections of the test correlated significantly with the total score (five of the six major sections at the 0.01 level of significance, the other at the 0.05 level) and sections apparently measuring similar abilities correlated highly, the Construct Validity was high. The results are presented in Table 7.6. The achievement of a moderate Concurrent Validity was indicated by the correlation of the score on the Achievement Scale with an external measure of ability: the end-of-year examination score for the Organic Chemistry paper. This correlation had a value of 0.353 and was significant at the 0.05 level.

Overall, therefore, the Achievement Scale had reasonable levels of reliability and validity.

(4) Results of the Achievement Scale

Overall the scores on the test were low, indicating that the level of student mastery of NMR was overestimated. The test was simply too difficult for most students and as such demonstrates a significant failing in its construction.

The tendency towards low scores leads to a rather homogeneous set of results, which generally makes correlations with external measures low and can often decrease internal consistencies. Coupled with the differences, both in administration and between the student groups, the deduction of firm conclusions from the various scores can be difficult. One external measure available was the percentage score in the end-of-year examination for the Organic Chemistry papers, although, unfortunately, the Honours students sat a different paper from the majority of students.

The data in Table 7.7 summarise the results of the test by section and list the three groups of students involved: users, "non-users" (students from the same group who did not use the teaching package) and the Honours students.

(5) Meaning of the Achievement Scale

The overall difficulty of the test means that any conclusions are tentative. Comparing the Honours and Stage 2 classes does indicate that the former students are, as might be expected, more capable, as illustrated by the comparison of performances in the reasoning sections of the test (4, 5 and 6) with the recall sections (1, 2 and 3).

Table 7.6

Inter-Section Correlations in the "Test"

Correlation of Section Scores with Total

Section		Correlation
1	Multichoice/short answer	0.586
2	^{1}H NMR Shifts	0.466
3	^{13}C NMR Shifts	0.334
4	Deduction of a compound	0.589
5	Prediction of ^{1}H spectrum	0.787
6	Prediction of ^{13}C spectrum	0.820

Correlations of Similar Sections

Sections	Correlation	Significance
2 and 3	0.378	0.05 level
5 and 6	0.744	0.01 level

Table 7.7

Mean Scores in the "Test"

Section	Possible	Users	Non-Users	Honours
1	36	14.5	13.3	13.1
2	20	5.9	4.7	4.9
3	20	6.5	4.5	4.5
4	20	10.9	4.5	11.6
5	20	7.6	2.0	10.1
6	24	8.4	4.5	7.4
Total	140	53.8	33.5	51.0
Exam	100	65.9	65.2	67.2

The depth and perception of written comments received with the Attitude Scale confirms the comparison between the groups.

Of interest, however, are the higher scores of the Stage 2 users of the teaching package over the non-users from the same class, even though the mean end-of-year examination scores are comparable. In addition, the users of the teaching package seemed to have more acceptance of ^{13}C NMR than the other students. This is attributable to the teaching system, since exposure to NMR outside of the teaching package is largely limited to ^{1}H NMR.

Further analysis of individual results did indicate that exposure to the teaching package did have an effect on test performance. Given that the major effect in the score on the "test" was likely to arise from the ability of the student, it was decided to study the combination of "test" score, ability (measured by end-of-year examination) and time spent on the computer. The various correlations between these three factors is contained in (Table 7.8).

The correlation between the time spent using the teaching package and the score on the Achievement scale was not significant (0.05 level of significance was at 0.4973). It is, however, possible that a larger effect was masked by the tendency of the more able students (as measured by the examination score), who tended to achieve higher test scores, to spend less time on the teaching package, as evidenced by the negative correlation. This last tendency was possibly a result of the imposition of required use of the package, with the more able students spending what was

Table 7.8

Effects of time spent on the teaching package

Correlations for Computer System Users

"Test" score and time spent	0.209
"Test" score and "examination"	0.482
"Examination" and time spent	-0.231

Comparison of Estimated and Actual Scores

	All Students	Computer Users
Estimated Mean	49.2	54.2
Actual Mean	49.3	52.8
Estimated Standard Deviation	20.9	21.2
Actual Standard Deviation	9.4	9.2
Correlation	0.478	0.593
Level of Significance	0.01	0.05

thought to be a minimum amount of time using the computer without them having the desired motivation.

A relationship between the time spent on the teaching package (T) and ability, as measured by the end-of-year examination result (E), was suggested by the above interactions. A simple representation of this interaction was thought to be:

test score = a x E + b x T + c x E x T,

where a, b and c were constants. Estimating test scores with a=0.664, b=0.196 and c=0.001, produced favourable results (Table 7.8). As a comparison, the best result for a linear relationship between the examination score and the test score, with constant a set to 0.742 and constants b and c to zero, obtained a correlation of 0.359, which was significant at the 0.05 level. A correlation of 0.607, significant at the 0.02 level, was obtained for the students who used the package (a=0.692, b=0.123 and c=0.001).

The inclusion of a factor for the time spent on the teaching package resulted in an increased correlation. This suggested that time spent on the package had a positive effect on test performance.

(6) Overall Summary of the Achievement Scale

Assessing the impact of the teaching package in terms of an increase in performance on a test is a task fraught with perils, even without the additional difficulties outlined. The motivation for students to complete the test was a hard factor to assess and although most attempts did appear adequate, there were indications that some results did not reflect the true ability of the students. Having to

make the teaching package compulsory also highlighted the problems with its use. It is doubtful that the desired high levels of motivation for the successful use of the package were achieved. In addition, whether the two variables used in the analysis (the final score in the Organic Chemistry paper and the time spent on the computer) were directly proportional to basic knowledge and ability of the student on one hand and the information and understanding imparted by the teaching package on the other was open to question.

In the administration of the scale the difficulties in assessing the benefits of teaching with CAL packages in terms of quantitative increases in ability became apparent. It has proved possible to measure significant improvements in performance using computers, although mainly in simpler studies. The effect of a more general CAL course was assessed by Mihkelson (1985). The study, which involved first year Chemistry students, found "a marked improvement in the performance of the CAI group" in the end of year examination.

There were indications that the use of the teaching package was of benefit to students, as measured by performance in the Achievement scale. The best examples were with students of moderate ability, who appeared to gain considerably from using the package. The fact that those students willing to make good use of the teaching package showed a marked improvement was, perhaps, the most significant result of the Achievement scale. Ayscough (1976b) noted a similar effect.

Chapter VIII

GENERAL DEVELOPMENT OF A TEACHING PACKAGE

In the creation of the NMR teaching package it became apparent that there were three aspects essential to the development of any computer teaching system. First there is the preliminary planning and careful identification of the topic to be studied. The second stage concerns the manner of presentation of the material and the third stage is the analysis of the feedback both from students using the package and from fellow teachers. The three stages are not however independent. The package development may be viewed as a cyclic or iterative process. Content is assessed and programs or lessons written. The results are then exposed to a variety of users and will undoubtedly result in a reassessment of the package, followed by modification and re-exposure.

1. PLANNING

It is essential in the development of any CAL exercise that both its general objectives and the users for which it is targetted be clearly identified. Once each has been established, specific objectives may be formulated, based upon the material to be presented.

Typically objectives will be stated in the form of the acquisition, by students, of specified information and are usually measured by the mastery of a number of skills. It

is important that these objectives be quite clearly defined in the early stages of development, otherwise there will be inefficient use of resources and very likely production of inappropriate material. The more general a lesson is made, broadening its applicability to a wider range of students, the more difficult it will be to produce and the less its likely impact.

Once the aims of the exercise have been established, the detailed material may be gathered. In the construction of the NMR teaching package, material was assembled from a number of sources (Chapter II), guided by expert opinion. Producing material tailored to the objectives and to the abilities of students was then a matter of careful elimination of much detail, while maintaining internal consistency.

Users are generally difficult to plan for, since they often vary widely in terms of preparedness. Although CAL packages are seen not so much as a means of presenting completely new material (but rather as a part of the complete educational process in Chemistry), it has proved to be reasonable to assume students have little background in the subject. In this way it is possible to cater for the fullest range of students.

2. PRESENTATION OF MATERIAL

There are three important techniques which can be employed in the presentation of material in computer teaching programs. The terms "lecture", "practice" and "discussion" are used to describe these techniques.

The lecture style is used to present all of the necessary background information and may also be used to review specific portions at the user's request. Practice generally involves significant interaction between user and computer and may often be in the form of a simulation of a Chemical process. Games may also be used for practice, as may question-and-answer (drill and practice) sessions (Eisele, 1979). Discussion involves more dialogue between user and computer than is present in the lecture type of presentation, although the two styles may overlap. Similarly, the question and answer session used for practice is essentially a discussion.

A complete teaching exercise should contain a blend of all three styles of presentation that seems appropriate to the topic. Generally the more difficult the topic, the greater should be the amount of practice and discussion. However, there should be some separation between the various components, so that each may be accessed relatively easily, as required. For example, there is little value to be gained from including a detailed, lengthy practice exercise as part of a discussion, if the user is not able to access that practice exercise independently. Experience suggests that users would be reluctant to use such an exercise more than once, however effective the practice part might be.

Overall, an effective teaching package should contain a variety of styles and be modular in design. In addition it should be relatively self-contained, with few if any references to external information, and with as little reliance as possible on student prior knowledge.

Further discussion of the detail and importance of each of the three important types of presentation is made below.

(1) Lecturing

It is likely that some sort of presentation of background theory, probably in a textual form, will be included in a teaching package, if simply for reasons of completeness. This style of presentation is referred to as the lecture style.

The lecture style may prove to be a useful point from which to begin the development of a teaching package. Certainly the need to include all of the background material in the tutorial exercises (the lecture component) of the NMR package served to clarify the objectives of the package. In addition early exposure to student users (as part of the "feedback" process) indicated the areas of the subject with which students had difficulties. This in turn indicated directions for the development of later parts of the package (the practice and discussion exercises).

There is, however, some opposition to the lecture approach in Computer Assisted Learning, on the grounds that simple "page-turning" text presentation is available in, and furthermore should be left to, text books. Some authors have suggested that a computer cannot function in the place of a human lecturer and that CAL is simply "computerised programmed instruction" (with the implication that this is totally undesirable), although both arguments have been refuted (Ayscough, 1977). While the inclusion of a large amount of purely textual material may in some cases be no

improvement upon the presentation available in, say, a text book, this does not always need to be the case.

In the teaching package, the two programs included to provide the required background information formed a vital part of the whole exercise. Access to on-line material proved to be an important feature, allowing students to receive, relatively easily, information tailored to their needs without the distractions and frustrations of referring to often irrelevant and possibly unavailable external sources. Although the material presented was largely textual, the use of diagrams (often including animation), the attention given to screen layout, the organisation of the presentation and the availability of a review facility advanced the tutorial programs considerably from the "page-turning" category. In addition, student users were able to control their own rate of progression through the programs, since there were frequent pauses allowing the entire display to be studied, before continuing or reviewing previous displays.

Interaction between student and computer is a subject often raised during discussion of Computer Assisted Learning. It is implied that the inclusion of significant interaction, usually by question and answer, is important to the success of CAL exercises (for example, Caldwell, 1980 and Gagne, Wager and Rojas, 1981). Indeed there can be little doubt that the reinforcement of material gained by effective interaction is an aid to learning (Dence, 1980 and Cohen, 1983). However in the lecture (review) style of exercise, excessive demands upon the user are inappropriate.

In the main body of the tutorial section of the teaching package, the continue/review choice and some other simple requests for input represented the only two-way interaction between the computer and user. There is no need to force students to understand every detail. If the major points are presented in a memorable fashion, if there is easy access to the minor details and if the remainder of the teaching package is designed as a complement (usually by practice and discussion), then the objectives of the exercise will eventually be achieved.

(2) Practice

Practice exercises are often included within teaching programs to aid understanding of the topic under study. Such practice exercises may take many forms, varying from drill-and-practice, in which students are given various problems to solve, to simulations, in which users may control variables in a generally simplified reproduction of a Chemical process. Games may also be used to achieve similar results (for example Bork, 1975a and Eisele, 1979), by using a generally un-real (but often exciting) exercise, based upon the chemical principles being expounded, with the hope that users will become accustomed to those principles through repeated use.

In the teaching package the "practice" was generally closer to the simulation style, with drill-and-practice being regarded as a subset of "discussion". Practice was therefore based upon the illustration of the underlying theory, by its application to a simple, complete exercise, which may be repeated with differing results each time.

With this illustration and repetition it was expected that users would gain the desired understanding.

Of greatest importance in the design of a practice exercise is the overall lesson context in which the exercise is placed. How the practice is achieved and what is being practised should be relevant to the material contained in the remainder of the package, since poor practice leads to the establishment of poorly-learnt or understood material (Cronbach, 1963, p.284). A practice exercise should therefore be undertaken in conjunction with some theoretical principle, which is made clear to the users. As noted previously, however, the modularity of a teaching package should be preserved as far as possible, so that there is easy user access to the desired activity.

In the teaching package the two practice exercises had complementary roles (Chapter IV). The first provided the opportunity to practise analysis of simple proton NMR spectra and gave direction for the second, which allowed students to create spectra and then to analyse them.

It is important also to appreciate the purpose of the practice exercise. With a clear goal in mind students can retain an appreciation of the total task at the same time as attending to the immediate details. Too many distractions from this overview tend to reduce the effectiveness of any exercise and for this reason practice exercises, especially of the simulation type, need to present a result that is quickly developed from student input. This has two general implications. Firstly, since interaction between student and computer is important, entry of data by users should be

as simple and yet as significant as possible. Secondly the model upon which the exercise is based should be simple, so that student attention is not lost as the results are being calculated.

There should be as few occasions as possible on which entry of information is required, and on those occasions a minimum of keystrokes should be required. Restricting the choice of options to those offered in a list (menu) is usually effective, provided that the list is short and displayed upon the screen as the choice is made. Complex exercises with large sets of instructions would seem generally to be ineffective as aids for practice and would be rather more suited as tools for research or demonstration. It should also be noted that students seem to pay only cursory attention to detailed instructions and therefore reliance should not be placed upon their use. Instead, instructions presented at the commencement of an exercise should be of a general nature to convey an idea of its overall purpose, and may be used primarily to conceal computer activity, such as initialisation.

(3) Discussion

Discussion exercises are those exercises that are not obviously intended as lecture or practice sessions. They range from simple question and answer (drill and practice), with or without any real presentation of background theory, to full dialogue, where user and student converse almost as equals. For a Chemistry teaching package, in which concentration on interpretation and opinion is not a significant

initial requirement, it would seem most reasonable to tend toward the simpler style.

As with the other styles of presentation it is important that a discussion exercise has clear author-defined objectives and a student-perceived role. The purpose of a discussion exercise may be to test student recall of material and aid in correcting any misconceptions, or it may be to aid in the review and extension of presented material. In the teaching package discussions were used in three ways: to accompany the tutorial programs in the guise of simple sets of questions, to present information (for example the NMR MACHINE lesson), and to round out the whole package, as in the TUTORIAL lesson.

Author objectives of discussions should usually be more than simply "to test student recall", although this may be a useful enough device for the student. In the teaching package a discussion exercise was associated with each of the lecture programs. These exercises took the form of a series of questions, but had the aim of exposing students to important material contained in the tutorial programs. In addition the exercises appeared to fulfill a real student expectation that some sort of test would accompany the package. Many of the factors involved in the planning of discussions may be found in Gagne et al (1981).

The general role of the discussions in the teaching package was to encourage students to think about aspects of NMR. In simple terms this is achieved by presenting material and asking questions about that material (or extensions of it). Setting the level of challenge in a

discussion is perhaps one of the most difficult aspects of its construction, since a high level of difficulty may discourage users, while a low level may not provide sufficient stimulation.

Again the objectives of the discussion provide an indication of the appropriate level. Questions of variable difficulty were included in the exercises accompanying the tutorial programs to focus attention upon important aspects of the theory, to allow students to demonstrate knowledge and to present that theory again. In the more serious discussions, questions were generally aimed both at maintaining student interest throughout the discussion and at promoting retention by stimulating thought about key points.

A discussion exercise is characterised by a reliance upon a significant amount of "verbal" interaction, with students entering words and sentences using the keyboard. It is important that this interaction be handled efficiently and accurately. The amount and detail of material presented and the questions asked in a discussion, are highly dependent upon the objectives of the lesson (Chapter VI). Most recommendations in the literature for the presentation of material are adequate (Jay, 1983), although few authors note that the verbal part of the display should be constructed with the convenience of users in mind. It should be brief, well-spaced and centred in the screen, with line breaks at logical places in the sentences and not simply where convenient. Courtesies, such as keeping the question displayed upon the screen while it is answered, are

also important. These approaches were adopted throughout the teaching package.

Analysis of student responses is the second essential capability of a discussion exercise. Allowing a free-form response to a question greatly increases the author's problems and may often be a factor in poor instructional design. Formulation of carefully worded questions, which request single-word or short-sentence answers, results in the entry by students of more easily analysed responses and also minimises the number of student typing errors. An Author language (Chapter V), with its built-in answer matching facilities, is a distinct advantage here. In the construction of the teaching package, it was considered important to make the reaction to student input low-key, using simple affirmative responses for correct answers, mild replies for incorrect answers and neutral responses for other answers. A small range of affirmative responses was used for correct answers. It was decided not to use a wide range of enthusiastic responses, since students may associate different degrees of correctness with different responses (Nievergelt, 1980). It was occasionally observed that some students became more interested in the responses than the material, a phenomenon also noted by Caldwell (1980).

In the teaching package, students were generally given remedial help upon entering an incorrect answer and were allowed one further attempt at the question, in general agreement with Caldwell (1980), although differing circumstances imposed different restrictions. The correct

answer to the question was eventually displayed in full in all cases, despite suggestions to the contrary (Cohen, 1983), since this information, rather than a fine judgement on the correctness of the student answer, was judged to be the most important consideration.

It has been suggested that the inclusion of branching, with detailed remedial help for students, leads to more effective discussion exercises (for example, Dence, 1980). Branching was employed in the teaching package, although only in the simple form outlined previously (an incorrect response received some guidance before the question was re-asked). The material that was the subject of the question was displayed in full to all students and not just to those answering incorrectly. The importance of this full display was perceived during early testing (Chapter II).

3. FEEDBACK

As has been stated, it is important to obtain the ideas of both experts and student users on a teaching package. This is because it is obviously necessary to build a package which presents the required information not only in a correct and adequate manner, but also in an interesting and effective one.

Experts on the chosen topic should be involved early in the planning stages. It should be noted that it may not be appropriate for the Author of a package to be an expert in that topic. If he is, there may be sacrifices in content, quality and flexibility for exigencies of programming. It is the task of the Author to structure the

material necessary for inclusion in the package and to decide how it is to be presented. This usually involves the deliberate omission of material which might otherwise have be included by an expert, in order not to overtax the attention span of student users.

As the above example illustrates, there are a number of conflicting influences affecting the initial design of a package and, indeed, its entire construction and subsequent refinement. The validity of decisions made about these conflicts may be assessed by frequently obtaining feedback from both expert and student user. It became apparent during the construction of the teaching package that it would prove to be a serious mistake to ignore such feedback.

Feedback from student users may expose problems in the actual programming details, even after an exercise has been extensively tested. Of more importance, however, is the fact that users soon make obvious the areas of the package that should be improved and will often indicate the direction future development should take. Careful attention must be paid to all user comments and difficulties, since if an exercise is not well-received and is not moderately easy to use it is likely to be under-used and hence of limited value.

Contact with student users should include personal attendance at user sites, since most of the significant student reactions to a presentation seemed to occur when they were actually using the computer. However in such situations caution must be exercised in interpreting student reactions. A complete teaching package of the sort

described in this project is designed for student users, either singly or in small groups, with little external input. There are three important consideration to bear in mind when observing student users. The first is that any distracting external influences may reduce the effectiveness of the package. Any observation should be discreet, since the behaviour of student users may be altered if they feel under close scrutiny. The second is that the motivation of a student user is an important factor in the effectiveness of the package for that student. Motivation also has an effect upon the reaction to an exercise, with less-motivated students generally being less satisfied with the form of the display. The third consideration concerns group influences on student reaction. The reactions of individual users are usually a more reliable guide than group reactions.

4. OTHER CONSIDERATIONS

(1) Hardware

Many authors have addressed the questions involved in the choice of hardware. These questions have ranged from the general, such as the desirability of a graphics capability, to the specific, such as the merits of particular brands (Moore et al, 1980a).

While it is clear that there is no uniquely suitable microcomputer, there are however a number of requirements a machine must possess before a successful package can be developed. The most important of these are that the computer is easy for students to use and that it possesses a good graphics capability (Thorn, 1980). Also of importance

are the physical transportability of the machine, the range of languages it supports and the amount of software available for it.

Since graphics is of central importance in a teaching package (Bork, 1975b), any computer used for CAL work must have at least medium resolution graphics (200 x 300 pixels), preferably integrated into the computer architecture. Such a graphics ability needs to be freely available to the Author. A potentially valuable asset would be the inclusion of colour (Kidd and Holmes, 1982 and England, 1984). Colour may be used to improve a screen display by highlighting important features and enhancing overall presentation. The monitor must however be of sufficient quality so that the legibility of text is not unduly sacrificed. It is also necessary to ensure that impact is not impaired or lost when a colour-using program is used with a monochrome display.

The computer chosen must be relatively easy for students to use. Given that some users are uneasy at the prospect of using a computer, any requirement for expertise with its use is clearly unacceptable. At most students should be expected to insert diskettes into disk drives and to turn on the machine in order to be able to access teaching material. The teaching package was confined to two disks and required no hardware intervention by student users. Cavin et al (1980) adopted a similar strategy.

Another physical constraint upon the computer is that it should be relatively easy to transport, especially if there are few available machines. Students tended to use the teaching package when it was convenient, and the

mobility of the computer, allowed it to be brought to them, in the teaching laboratory (Chapter VII).

(2) Languages

As with the choice of computer, the suitability of a wide range of microcomputer languages for CAL work has been discussed (for example, Schuyler, 1979). There is no single language suitable for the production of all CAL material. The choice of a language for a teaching package should therefore be dependent upon the purpose of that package and, indeed, there may be a need to use more than one language.

As has been indicated, a self-contained teaching package is likely to contain three styles of program: lecture (review), practice, and discussion. It seems likely that simulation (practice) exercises will necessarily require an all-purpose computing language such as **Pascal**. Lecture exercises might also require the generality of such a language. However at least some of the discussion exercises could be implemented using an Author language, with a significant increase in convenience for the author.

Development of a CAL package should therefore be based upon a sufficiently powerful, general-purpose language, with any other languages used able to be incorporated into the package. It must however always be remembered that users are the prime consideration. Ease of development at the expense of user-convenience is to be avoided. Similarly, if the use of an interpreted language (such as the BASIC available on many microcomputers) would result in a significant reduction in performance when compared with a compiled language (such as **Pascal**), then it should not be

considered, even though it may have other developmental advantages.

Other considerations involve the ease of maintenance and transportability of software. Generally speaking the common "natural" language of many microcomputers, BASIC, is not especially easy to maintain and may be difficult to transfer to another computer. It does not therefore seem to be a suitable choice (Helmers, 1978). Languages, such as **Pascal** and FORTRAN, are generally superior in terms of construction (and therefore maintenance) and are available on many microcomputers. UCSD **Pascal**, a version of which was used in the teaching package, has many supporters as a language (Wakerly, 1979, Alpert, 1978, Mundie, 1978). Certainly in the teaching package this language performed satisfactorily.

(3) Students

Differences in individual students will inevitably result in different reactions when they take part in any activity. In constructing a teaching package it is usually difficult to take full advantage of the individuality of student users. Experience has shown that the Author should seek to avoid anything that might provoke a negative reaction from students. This generally means that the Author has to keep close control over the presentation and, as has been previously noted, should maintain a close personal observation of students using the package.

Qualitative indications from testing throughout the development of the teaching package suggested that students did appear to gain considerably from the programs on offer.

When such use was optional, the users were generally well-motivated and interestingly there seemed to be a tendency for them to be of higher academic ability. In compulsory use of the teaching package the range of motivation was wide. Those with low motivation received minimal benefit from their short sessions with the computer. Generally there were fewer highly-motivated users than was the case with the optional use of the package and the students with the lower motivation tended toward the average to high level of ability. There appeared to be two trends involved in the compulsory use of the package, with the more able students spending what they thought was the minimum allowable amount of time, and the less able students feeling that they could afford little time with the machine. Analysis of the data for the Achievement scale (Chapter VII) supported this belief.

Having noted that motivation has an effect upon the impact of a teaching package, much depends upon the circumstances of its use, rather than its actual content. The Author may, by following previously-noted recommend-ations outlined for example in Gagne et al (1981), enhance motivation by creating the initial attraction and maintaining interest throughout the course of the package (Caldwell, 1980).

Allowing for variations in the personality of students generally leads to a more impersonal approach as noted in Jay (1983) and Nievergelt (1980). The personality of users will often govern the reaction to other stimuli, such as scrutiny. Many students appeared to feel extremely

uncomfortable when under obvious observation and this generally appeared to have an adverse effect upon the session. Removal of such disturbances is a matter of courtesy, as much as anything.

The teaching package was designed to be used by one student at a time. Users in groups may react differently from when they are on their own. There may be some beneficial effects on learning, since explanations of both material and program instructions are usually forthcoming from other group members and there is often helpful competition. However, sometimes the group moves too quickly for some members, causing some loss of interest and impact and thus losing one of the primary advantages of the computer, namely individually-paced instruction (Dence, 1980). Dominant group members may also deprive other students of benefits by monopolising the computer, with similar negative results. The most common effect of groups is the decrease in freedom of responses, especially in the more difficult exercises.

Chapter IX

SUMMARY AND CONCLUSIONS

The overall aim of this research was to find a method of effectively implementing CAL in Chemistry, using a microcomputer. In a physical sense this involved the documentation of a compact and effective CAL package, which allowed students easy access to relevant material upon a topic in Chemistry. Measurement of the effectiveness of that package was also an essential part of the research.

1. THE TEACHING PACKAGE

The research involved not only the construction of a physical teaching package, but also the acquisition of techniques and the creation of tools for the construction of other CAL exercises in Chemistry. The many considerations involved in the actual construction of the package have been presented, as have many of the techniques for its design. It was not the purpose of this project to create a perfect package, if such was achievable, but instead it was to provide a model upon which to base further development of teaching packages.

Briefly, the teaching package consists of a number of programs and lessons which treat the topic of Nuclear Magnetic Resonance from a variety of viewpoints. It was considered essential to include an easily-used source of background material, programs to allow practice and

discussion exercises to encourage further consideration of NMR. Advice concerning the merits and use of each of these means of presentation has been offered in some detail.

Lesson planning and student feedback has been examined and more fundamental concerns of CAL Authors, such as the choice of programming language, have also been discussed.

2. A PLACE FOR COMPUTER ASSISTED LEARNING IN CHEMISTRY

Education in Chemistry at University level is largely based around lectures, through which the essential material is presented, often in outline only, to students. Laboratory sessions allow students to practise essential technical skills and to relate theory to actual experimental conditions. Laboratories also allow more personal contact to be made between students and staff. In the many cases where essential knowledge of material is presented imcompletely in the formal part of the course, students are expected to research the remainder independently.

In a study of attitudes "towards using computers as instructional aids", Offir (1983) investigated the attitudes of "instructors" (tutors and lecturers) and students and the interaction of these attitudes. Interviews, questionnaires and observation were used to assess these attitudes. Offir noted that during interviews the majority of instructors mentioned that "the aim of teaching at University is to develop the capability of self-study and to improve student understanding of the subject matter." However, in contrast, he noted that students felt that the purpose of University was "to supply information" and that, when considering the

differences between students and instructors, that "the actual situation is closer to the opinions of students."

Offir also attempted to determine the preferred method of instruction for students. Lectures, in which the presentation of material was direct, rated highly, while CAL programs, written in accordance with the recommendations of the instructor (with more emphasis upon understanding), rated poorly.

Not all of the findings of Offir's study are directly applicable to this research, however. It was apparent, firstly, that Offir's study of attitudes was more general ("mention the preferred method of teaching") than that undertaken in this research. Secondly, the objectives and use of his CAL programs did not appear to be well-defined and, as it has been shown, the effectiveness of computer teaching packages is dependent upon the clarity of objectives.

In the assessment of attitudes undertaken in this research (Chapter VII), student attitudes to Computer Assisted Learning were essentially neutral in response to statements equivalent to those used in Offir's study ("I would not use a computer in preference to any other method of learning"). Such a response is more likely to be an indication of avoidance of the subject (the "don't know" choice) or that the statement is inappropriate or vague, than it is to be an actual judgement.

More specific statements gave a better indication of student attitudes towards CAL and how it should be used as a part of Chemistry (Chapter VII). The statement indicating

that "lecturers should utilise CAL to complement lecture courses", received support from both students who had used the teaching package and those who had not. In addition, written comments reinforced this opinion, with the idea that CAL was perhaps best at reviewing and expanding upon material presented in lectures. One student commented that the computer was good for "teaching rather than lecturing". It is apparent that CAL may represent a method of achieving the aims stated by "instructors" in Offir's study, in that it gives students the opportunity to gain understanding of material through individual study.

Computer Assisted Learning in Chemistry should therefore be used as a complement to the already existing parts of the educational package. It has already been reported that CAL, in conjunction with traditional methods, has achieved significantly improved results over each method used individually (Dence, 1980). When properly managed on a larger scale there could be considerable benefits for both lecturers and students. Comprehensive collections of CAL packages would enable lecturers to concentrate upon the applications and ramifications of the topics, rather than all of the details, while laboratory demonstrators would be able to refer students to relevant material as necessary. In a recent study (Whiting, 1985) CAL material took the place of tutors in a course with "no downgrade in performance". In fact it was claimed that the CAL tutor "is superior in promoting mastery" when compared with a human tutor.

Each CAL package should provide a consistent (rather than complete) coverage of a topic, tailored to a specific group of students. In this way it may be used as a reference by students seeking to increase understanding or to review material, rather than as a means of presenting large amounts of new material. Libraries (or the lecturers themselves) would remain the ultimate source of information.

While the use of a computer in almost any part of Chemistry may be regarded as Computer Assisted Learning, as has been noted, it is important that its use have a clear role in the educational package. It is for this reason that emphasis has been placed upon complete teaching packages, such as the one constructed in this research.

3. THE FUTURE OF CAL IN CHEMISTRY

It is hoped that Computer Assisted Learning based upon microcomputers will be implemented sensibly and will be used widely as an educational tool in Chemistry. CAL packages, such as the one created in the course of this research, should be of considerable benefit in achieving this end.

The NMR teaching package appeared to be successful in increasing the achievement of students who would be most likely to take advantage of the introduction of such packages. The more motivated students said that they gained significantly from the CAL package and did indeed appear to have done so. Improvements in achievement using CAL have been widely reported in many areas (Dence, 1980, Mihkelson, 1985). In addition, the attitudes of students towards CAL appeared positive, whether they had encountered the teaching

package or not. Students asked for more freely-available CAL, covering more topics. Again similar attitudes have been reported elsewhere (Cavin et al, 1980).

Attitudes of lecturers in Chemistry are harder to assess. For example in Offir's study of the differences between student and "instructor" attitudes to CAL (Offir, 1983) "instructors" displayed a positive attitude. However none made use of the CAL programs even though these were able to be modified to the personal requirements. Ayscough (1976a) noted a similar phenomenon, where apparently positive attitudes do not translate into actions. Therefore, while there are many supporters of the use of CAL in Chemistry, there are enough lecturers sufficiently unsure of, or opposed to, this method of delivery, to hinder its inclusion as a viable teaching method. Exaggerated claims about the value of CAL and both insufficient planning and experience in the production of some software have already produced a significant reaction against CAL using microcomputers (Pehrson, 1985). This may be analogous to the reaction against earlier CAL material.

Despite reservations in some quarters, however, it seems probable that the use of computers for teaching will inevitably gain wider acceptance, if only through the increasing exposure to computers. The advent of software that is accepted by students and is demonstrably effective (especially to instructors) will hasten this process. While there is the possibility that "the present low standard of CAL material will become <u>the</u> standard" (Bork, 1984), it is

hoped that this study provides guidelines for raising the standard of future CAL material in Chemistry.

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Much of the background material upon Nuclear Magnetic Resonance for use in the teaching package came from text books. The following were especially useful: Abraham and Loftus (1979, particularly p.1-80), Becker (1980, p.1-107), Bovey (1969, 1-27), Breitmaier and Voelter (1974, p.1-37), Leyden and Cox (1977, p.1-50), and Williams and Fleming, (1966, p.77-129).

The Achievement scale was constructed with regard to a number of references. Anastasi (1976) was a good general text, Heywood (1977) was an excellent source of material and Cockburn and Ross (1977), Cronbach (1961), Popham (1978), Rowntree (1977) and Tittle and Miller (1976) were also useful.

Material for the construction of the scales was also obtained from a number of sources. Oppenheim (1966) proved to be excellent, while Anastasi (1976) and Shaw and Wright (1967) were helpful.

APPENDIX A

CONSIDERATIONS IN BUILDING THE TEACHING PACKAGE

The teaching package consisted of a number of programs and data files stored on two 5 1/4 inch diskettes, for use with a dual-disk drive APPLE II computer with at least 64 kilobytes of memory. The manner of deposition of these files and programs on to the disks was an important consideration. It was governed not only by the available space, but also by a consideration of the amount of disk activity, since excessive time spent reading from and writing to disk may have a negative effect on student users. A description of the necessary files and programs in the package and of their placement on the disks is included in this section.

There were a number of additional programs of a utility nature that were not included on the teaching package disks. These programs were used in the construction of the various parts of the package. The most obvious of these was the analyser for the MASTER language, which was designed to convert source lessons into interpretable files.

1. CREATING THE PHYSICAL NMR TEACHING PACKAGE

The creation of the physical teaching package was a matter of arranging three groups of files (the APPLE PASCAL System files, the MASTER lessons and the larger programs) on to the two diskettes. A single disk version of the NMR teaching package was also constructed.

(1) The System Files

Various PASCAL System files were necessary on the "boot diskette" (the disk placed in the first disk drive when the machine was switched on) to prepare the computer for the running of the PASCAL System. Of the System files (Table A.1) only two were of interest: SYSTEM.LIBRARY which contained the PASCAL Functions, including the graphics routines, and SYSTEM.CHARSET which held the shapes of the characters which appeared on the graphics screen.

One file with the prefix "System." was not strictly an APPLE System file. Although a feature of the operating system, SYSTEM.STARTUP was, in fact, a program able to be written by the Author of any system. This program was executed automatically when the "boot" process was complete. In the case of the teaching package, the purpose of the startup program was to check for and, if necessary, activate any lower case capability of the computer and to then execute the program RESTART.CODE (Table A.2).

The restart program contained the teaching package main menu and allowed access to all other programs of the package. If no choice from the menu was made within a certain time, the overlays from the NMR MACHINE lesson (Chapter VI) were slowly presented. When one of the options in the menu was chosen, the appropriate program was started. Upon completion the program RESTART was again invoked to continue the process. In the case of abnormal termination of a program, the computer would "reboot", execute SYSTEM.STARTUP and hence RESTART. Student users therefore faced a closed system.

Table A.1

APPLE System Files

Name	Size (512 byte blocks)
SYSTEM.APPLE	32
SYSTEM.PASCAL	41
SYSTEM.MISCINFO	1
SYSTEM.CHARSET	2
SYSTEM.LIBRARY	24

Table A.2

Special System Files

Name	Size (1/2 kb)	Purpose
SYSTEM.STARTUP	2	Activate Restart.Code
RESTART.CODE	6	Teaching package menu

(2) The MASTER Lesson Files

The second and probably most important limiting factor was the need to minimise obvious disk activity. Although all of the disk accesses were necessary, the actual number was disguised somewhat by grouping related programs and files upon the same diskette. In this way several short disk accesses appeared to be a single continuous activity.

It was necessary therefore to place all of the compressed picture files and the MASTER Interpreter on the first disk since the MASTER lessons often required multiple short disk accesses to load the relevant picture files. This grouping (outlined in Table A.3) and the way in which the interchanges inside the individual MASTER lessons were handled (Appendix B) meant that the problem of disk accesses was rarely noticeable to student users.

(3) The Major Programs

With a considerable portion of the first disk occupied it was decided to place the four major programs (PART1, PART2, NMRSIMUL and NMRSPEC) and the accompanying files on the second disk. This arrangement may be seen in Table A.4. The six MASTER lessons were then placed onto the two disks so that roughly equal space remained on each (Table A.5). This allowed sufficient room for the statistics files, which were created at the completion of each of the MASTER lessons, to be saved. Each of the eight lesson files (two lessons were divided into two files) consisted of the three files produced by the syntax analyser.

Table A.3

MASTER Files

Name	Size (1/2 kb)	Purpose
INTERP.CODE	16	MASTER Interpreter.
LOGO.FSCR	4	Interpreter picture.
PIC.FSCR	4	Picture for PART1.TEST.
AROMATIC.FSCR	2	Picture for first part of TUTORIAL lesson.
COUP.1.FSCR	3	Pictures for the second part of TUTORIAL.
QUARTET.FSCR	1	
COUP.2.FSCR	3	
COUP.3.FSCR	2	
COUP.4.FSCR	2	
MULTIP.FSCR	1	
SPECT.FSCR	3	Pictures for the third part of the TUTORIAL lesson.
POINT.FSCR	1	
SHIFT.FSCR	1	
INDICAT.FSCR	2	Pictures for the fourth part of TUTORIAL.
OLLIE.FSCR	2	
REM.ETH.FSCR	1	
ENLARG.FSCR	1	
KBOARD.FSCR	7	Picture files for the KEY lesson.
KEY.1.FSCR	1	
KEY.2.FSCR	1	
KEY.3.FSCR	1	
KEY.4.FSCR	1	
KEY.5.FSCR	1	
KEY.6.FSCR	1	

Table A.4

Major Programs

Name	Size (1/2 kb)	Purpose
PART1.CODE	31	Part 1 of the Tutorial programs.
PART2.CODE	57	Part 2 of the Tutorial programs.
NMRSIMUL.CODE	25	Proton NMR simulation program.
NMRSPEC.CODE	27	Proton NMR analysis program.
TEXTFILE	9	Text of the NMRSPEC program.
MASTERFILE	1	Formulae of spectra for NMRSPEC.
FORMULAFILE	6	Comments to accompany the final answer in NMRSPEC.
SPECTRUMA	1	Data files for spectra.
SPECTRUMB	1	
SPECTRUMC	1	
SPECTRUMD	1	
SPECTRUME	1	
SPECTRUMF	1	
SPECTRUMG	1	
SPECTRUMH	1	
SPECTRUMI	1	
SPECTA.FSCR	2	Picture files containing the structure of the compound.
SPECTB.FSCR	2	
SPECTC.FSCR	2	
SPECTD.FSCR	3	
SPECTE.FSCR	3	
SPECTF.FSCR	3	
SPECTG.FSCR	3	
SPECTH.FSCR	4	
SPECTI.FSCR	2	

Table A.5

Remaining files on the first disk

Name	Size (1/2 kb)	Purpose
PART1.TEXT	12	The lesson accompanying
PART1.OP	2	PART1.CODE.
PART1.NODE	2	
PART2.TEXT	12	The first part of the lesson
PART2.OP	2	accompanying PART2.CODE.
PART2.NODE	2	
TUTORIAL.TEXT	12	The first part of the
TUTORIAL.OP	1	tutorial lesson.
TUTORIAL.NODE	1	
TUTE.CONT.TEXT	14	The second part of the
TUTE.CONT.OP	2	tutorial lesson.
TUTE.CONT.NODE	2	
TUTE.CONT.STAT	1	Statistics files produced by
PART1.STAT	1	MASTER lessons.

Table A.6

Remaining files on the second disk

Name	Size (1/2 kb)	Purpose
KEY.TEXT	8	
KEY.OP	1	The keyboard lesson.
KEY.NODE	1	
PART2.CONT.TEXT	12	The second part of the lesson
PART2.CONT.OP	1	accompanying PART2.CODE.
PART2.CONT.NODE	1	
MACHO.TEXT	10	
MACHO.OP	1	The NMR machine lesson.
MACHO.NODE	1	
INTRO.TEXT	12	The second part of the
INTRO.OP	1	tutorial lesson.
INTRO.NODE	1	
INTRO.STAT	1	
PART2.CONT.STAT	1	Statistics files produced by
KEY.STAT	1	MASTER lessons.
MACHO.STAT	1	

(4) Single Disk Drive Version

A version of the teaching package was also constructed for computers with only one disk drive. This version was necessarily spread over three disks, since the APPLE PASCAL System files needed to be accomodated on each disk. On booting the computer on any particular disk, a similar menu to that of the two disk version appears, with the available choices highlighted. Users choosing inappropriate options are referred to the relevant disk.

2. UTILITY PROGRAMS USED IN THE NMR TEACHING PACKAGE

The construction of the package proved to be dependent upon a number of programs that were not placed directly on the disks used by students. The most obvious of these were the text editor, used to produce the source files for programs, and the compiler, used to convert these files to executable programs. Early in the creation of the package it was sufficient to use a small number of programs to produce components of the package. For example, the tutorial programs (Chapter III) were originally simply large, single programs. As the complexity of the package increased, however, so did the necessity for sophisticated supporting tools.

There proved to be three areas of the package that required particular tools, although all overlapped somewhat. These areas were: 1) the production of MASTER lessons, 2) the creation of spectra for inclusion in the NMR Analysis exercise and 3) the preparation of "compressed picture files" for use in these areas.

(1) The MASTER Lessons

Apart from the MASTER language interpreter, development of MASTER lessons in the teaching package was based upon two utility programs: ANALYSE, to check the syntax of lessons, and TEACHER, to allow testing of lessons. In addition a third program, RECOVER, was useful in determining the impact and suitability of the lessons, by enabling analysis of statistics files produced by the MASTER Interpreter.

(a) The MASTER Analyser. As has been noted (Chapter V), the success of the MASTER language was based upon the conversion of the source lesson into an intermediate form, which was then interpreted when the lesson was used. The utility program ANALYSE performed the conversion from the source lesson to the "intermediate" form and was therefore of considerable importance in the development of the whole package.

Operation of the Analyser was designed to be as simple as possible. After the name of the lesson had been entered, the syntax of each of the lines was verified. Any error in syntax stopped the program, with the offending line and an appropriate message displayed. If the syntax of the lesson was correct, its internal consistency was assessed by considering references to the nodes. Any nodes not referenced were reported, but references to non-existent nodes resulted in an error message and failure of the analysis. The final function of the Analyser was to create three files containing the interpretable data. Possible incompatibility with the capacity of the Interpreter was

given if necessary, since ANALYSE was designed to be able to cope with larger lessons.

(b) The MASTER Author's Interpreter. Since all MASTER lessons required testing before inclusion into the teaching package, a version of the Interpreter to facilitate this testing became a necessity. TEACHER was simply a version of INTERP (the MASTER Interpreter), which allowed the name of an analysed MASTER lesson to be entered manually, rather than to be passed as a parameter by another program. In addition more diagnostic information was available, which enabled the function of both the lesson and enhancements to the Interpreter itself, to be monitored more closely than otherwise possible.

(c) Statistics File Analyser. The third utility program associated with the MASTER language was designed to retrieve the information stored at the completion of a lesson. This information, consisting of the responses (and the nodes accessed) entered by students using the lesson. The need for modification of the lesson, particularly in the wording or analysis of answers to questions, was often indicated by consideration of the data produced by this utility program.

(2) The Spectrum Analysis Utilities

The successful use of NMRSPEC, the ^{1}H spectrum analysis program, was essentially dependent upon the creation of the database of compounds whose spectra were to be analysed. A utility program, SPECSETUP, was designed to allow any author to extend this range of spectra. In addition another utility program allowed access to the

various data files containing the text associated with NMRSPEC. This enabled modification of the display of the teaching package program, without necessitating recompilation.

(a) Spectrum Creation Utility. A major utility program was designed to create and maintain the various files associated with the spectrum analysis program SPECSETUP. Three areas of input were required for each spectrum, corresponding to the MASTERFILE, SPECTRUM and FORMULAFILE data files. The necessary information was entered in response to a series of questions, which were designed to be as easy as possible to answer.

Entry of the formula of the compound was the first requirement: the number of carbon, hydrogen, nitrogen and oxygen atoms needed at most two keystrokes for complete entry (Figure A.1). This information was then incorporated into the master record file (MASTERFILE), which contained all of the formulae of the compounds in the database.

After entering the number of resonances appearing in the spectrum, information about each was requested. This information consisted of the Chemical Shift (to one decimal place), the multiplicity of the resonance, the fragment of the compound producing the resonance (selected from a list), and the neighbouring fragment or fragments as necessary (again selected from a list) (Figure A.2). When all of the resonances had been completed, the data was stored in a SPECTRUM file.

```
In the molecule how many....
CARBONS are there ? > [9*]

HYDROGENS ? > [10]
NITROGENS ? > [0]
OXYGENS ? > [1]
```

Figure A.1

Entry of a Chemical Formula using SPECSETUP

```
Peak NUMBER 2
Chem Shift > [2][6]

1> CH3 2> CH2 3> CH 4> BENZENE 5> OH
Fragment from list > [2]
Two or more equivalent CH2 groups?
      If so give how many > 1
Multiplicity > [4]

0> NONE 1> CH3 2> CH2 3> CH 4> BENZENE
5> CO   6> O   7> X   8> OH 9> N
Connected to ?> [1]


and connected to ?> [ ]
```

Figure A.2

Entry of neighbouring groups in SPECSETUP

The third part of the program was concerned with the entry of the structure of the compound portrayed by the spectrum. Although the analysis program required a compressed picture file containing the alternate structures, it was decided that rather than attempting to incorporate a graphics editor into SPECSETUP, only the comments associated with each choice would be required. The compressed picture could then be created as a separate exercise, by an expert in the task if necessary. The required name of the picture file was displayed. When the four sets of comments were entered, they were included in FORMULAFILE.

(b) Altering data files. The textual data for direct use by the spectrum analysis program, NMRSPEC, was stored in two data files FORMULAFILE and TXT, to enable more rapid access, allow easier editting and minimise storage space. A utility program, TEXTFRFILE, was designed to convert these files to and from a form able to be editted by the APPLE text editor. This proved to be especially useful in altering the textual display of NMRSPEC, allowing minor corrections to be made.

(3) Graphics Utilities

The development of many of the latter parts of the NMR teaching package was based upon the use of picture files, essentially previously-constructed screen displays. The use of such files enabled the MASTER language to be implemented successfully and greatly facilitated a crucial section of the NMR analysis program.

As has been noted (Chapter II), the ability to compress picture files was of considerable importance, since

both the number available and speed of display was increased. Of greater significance, however, was the development of utility programs to produce the actual screen displays. In addition, another utility program, a character set editor, was used to alter the character set contained in the APPLE PASCAL system file SYSTEM.CHARSET.

(a) Compressed Picture Files. The idea of compressing graphics screen pictures first appeared in 1983 (Green) and was intended for use with the APPLESOFT (BASIC) language. It was implemented in APPLE PASCAL (Blunt, 1983) and further extended for use in the NMR teaching package. When included as a part of the MASTER system, the use of compressed picture files became an important feature of the teaching package.

(b) Screen Editing Utilities. Developing screen displays for use with the various MASTER lessons proved to be a labour intensive task. For this reason a number of utility programs were developed.

The most important of these made possible the simple functions: line, box and circle drawing and the display of character strings, the conversion to and from compressed files and the dumping of pictures on to a printer. In addition it allowed a combination of keyboard and joystick input to control these functions, thereby greatly simplifying many tasks.

Two other programs were also of considerable value. GETSHAPE enabled any small portion of the graphics screen to be "captured" and repositioned or duplicated as required. PICIO was designed to capture a shape on the screen and to

convert it into a text file, which could then be edited by the APPLE PASCAL text editor. This allowed complex shapes to be altered more easily, by effectively increasing the resolution. The same utility was able to convert text files back into screen images, which could again be positioned or duplicated as a part of a new or existing screen display.

(c) Character Set Editor. As previously indicated, the APPLE PASCAL system file SYSTEM.CHARSET contained the data for the graphical representations of the ASCII character set. A utility program to edit this set enabled the appearance of the characters to be improved and the actual function to be changed in some cases. An extension of this idea was produced to enable larger-sized characters to be manipulated. Common shapes, such as the benzene nucleus, could then be easily displayed.

APPENDIX B

AN OUTLINE OF THE MASTER LANGUAGE

As with the STAF language, a MASTER lesson was defined as a collection of small units (Barker and Singh, 1985). These were referred to as "nodes", with each containing three essential components: (1) a definition, indicating the beginning of a new node and its associated name, (2) optional text for display on the screen and (3) operations indicating the next node to be accessed.

When a node is accessed, any associated text is displayed. Special characters embedded in this text can be used to modify the screen display with effects ranging from simple additions of characters to the overlay of designed screen images.

The operations may include the manipulation of numbers or analysis of student responses, for example, with the next node to be accessed being determined as a result of such operations.

Since this construction was less linear than that embodied in PILOT, the possibility of novice users adopting a "mediocre strategy" (Merrill, 1982) was diminished. Although considerable emphasis was placed upon ensuring that the Author was in control of a MASTER lesson, especially with the screen display, the basic outline of the language was designed to be as simple to use as possible.

1. NODES

To allow for maximum flexibility, node names were defined to be any combination of two letters, with the proviso that the first node in any lesson was "AA". Up to 100 nodes may be included in any lesson. Duplication of node names within a lesson results in an error and the termination of the Analysis program.

The format of a node definition is indicated by the construction: "#nn;*", where "nn" can be any combination of two letters. The asterisk is used generally in a MASTER lesson to indicate the end of an operation and, in this case, may be followed by text which is ignored by the MASTER Analyser, unlike its STAF equivalent. This text can be used to explain the purpose of the node, much as a comment may in a general purpose language.

To aid readability it has become standard practice to adopt some conventions in the naming of nodes. The most common include keeping the nodes in alphabetical sequence throughout the lesson, with groupings of similar names indicating closely-connected nodes.

The MASTER lessons for the questions associated with the tutorial programs have, for example, a similar layout. Nodes "AA" to "AZ" contain the introduction to the lesson, "ZA" to "ZZ" provide the utility functions, "BA" to "BZ" details question 1, "CA" to "CZ" question 2 and so on.

The "utility" nodes, which included the common request to "Press the key marked 'Return' to continue", were given the obviously different node names (ZA - ZZ) and a position at the beginning of the lesson for easy reference.

Readability was also enhanced, both by spacing the node names (e.g. CA, CE, CI....) to preserve alphabetical order when insertion of extra nodes proved necessary, and by including comments wherever appropriate in the lessons.

2. OPERATIONS

It was decided to limit the number of operations to allow the construction of a basic program to be as simple as possible, with much of the sophistication to be incorporated into the text associated with a node. Initially only operations involving the flow of the lesson were included (Table B.1), being analogous to the STAF operations.

The simplest operation for establishing the connection between nodes was the "Jump", which transferred lesson presentation to a nominated node. An extension of this principle was used in the "Subroutine" operation, which allowed the Author to indicate when each "Jump" in the "Subroutine" is to be performed. The "Subroutine" and "Return from Subroutine" operations have proved to be particularly useful where there is repetition, such as the presentation of prompts, involving a group of nodes.

In order to terminate a lesson an "Exit" operation was included.

(1) Jump to Node

The operation "JU" allows control to pass directly to a nominated node. The format of this operation is "!JU;nn*", where "nn" is a valid nodename.

Table B.1

Operations available in MASTER

Jump to Node	Pass control directly to a node. Example: !JU;BC*
Exit	Terminate the lesson. Example: !EX;*
Subroutine Jump	Pass control to a node. When "RS" encountered, pass control to nominated node. Example: !SR;$2ZDBC*
Return from Subroutine	Pass control to the next node in Subroutine list. Example: !RS;*
Match	Analyse response and perform an action. Example: !MC;@2* !JU;GC*0 HELP$$UNDERS !JU;GL*
Alter Counter	Define the value of a "counter". Example: !AC;%1=%1 + 4 *
Jump on Counter	Pass control to a node based upon the value of a "counter". Example: !JC;%1$2;LELA*

(2) Exit

Use of the simple "EX" operation causes termination of the lesson, with a message displayed on the screen for the user. In addition the student response file is saved. The format of this operation is simply "!EX;*".

(3) Subroutine Jump

"SR" allows a number of nodes to be accessed in order. From two to four nodes (the number indicated with the operation call) may be included, since the format of the "SR" operation allows a variable number of nodenames: "!SR;$xn1n2n3n4*". Here "x" is the number of nodenames and "n1", "n2", "n3" and "n4" are the actual nodenames.

A simple JU is made to the first node in the list, with the remaining nodes being pushed onto a "stack". Upon encountering each subsequent "RS", a JU is made to the most recently "pushed" node.

Up to eleven nodes may be held in the "stack" at once. Any attempt to store more than eleven results in the termination of the Interpreter. An error message appears on the screen along with a request for a demonstrator.

(4) Return from Subroutine

When the Interpreter encounters an "RS", a simple "JU" is made to the previously stored node (by SR). If no nodes had been previously stored, the Interpreter terminates (with appropriate messages). The format used with this operation is similar to that of the "Exit" operation: "!RS;*".

The "Return from Subroutine" operation is especially useful for often repeated nodes (such as the request to "press the return key to continue").

(5) Matching

Since the ability to analyse student responses was of utmost importance, the inclusion of a matching option was a necessity.

Typically an Author language requires the Author to provide a list of important words that will characterise a given response. These words are commonly referred to as "keywords". If the keywords are present in a response, it is assumed that the entire response is consistent with the keywords and some Author-defined action may take place. The STAF Author language supports a very powerful "match" command, which allows thorough analyses to be performed (Baker and Wilford, 1985). In practice it was noted the full range of options associated with this command was not often utilised and this fact was reflected in the design of the MASTER matching operation.

The MASTER matching operation may consist of several lines in a lesson, with an initial line indicating the matching to be performed and the remainder containing keywords and associated operations (to be performed on a successful match). The last line of an "MC" operation is always a single operation that is actioned upon the failure of all of the preceding keywords matches.

The first line of an "MC" operation has the format "!MC;@x" or "!MC;%x", with "x" being the number of following lines of operations. The form containing the "@" symbol

causes the Interpreter to request student input, as detailed below. The form with the "%" symbol uses the text of the last student input. The following lines except, as has been noted, the last, consist of an operation followed by a "severity" (either "0" or "7", as detailed below) and a list of keywords. An example is:

"!JU;GF*0 HELP$DONT$NO#IDEA"

which scans input for occurrences of the words "HELP", "DONT" (as in "DONT KNOW") and "NO IDEA" ("#" is used to mask a space).

If a match is successful with either "severity" the associated operation (JU, SR, RS, EX) is executed. In the previous example a "JU" to node "GF" would have been made.

The last operation associated with the "Match" operation is only accessed if there is no match with a list of keywords. The last operation may be one of the four previously indicated, or may be the "Jump on Counter Value" (JC, detailed below).

The number of sets of keywords, although arbitrarily limited in order to aid readability, may effectively be extended by using the "JU" operation in the last line to "jump" to a node (with no text), which has another "MC" (with the "%" option).

(a) Severity 0. This "severity" requires only that the keywords be present somewhere in the student input. Spaces in the keyword list imply that multiple words are required, while alternative keywords are separated by the "$" symbol. If the blank character is required in a keyword it may be masked with the "#" symbol.

The keyword list "THE$A CAT$DOG" will match "THE CAT", "THE DOG", "A CAT" and "A DOG", although it will also match a response with additional characters and words (for example "ANOTHER DOGMA").

The speed of this facility was achieved by utilising an intrinsic function of the APPLE version of UCSD Pascal.

(b) Severity 7. This "severity" may be regarded as an "exact match". Alternatives are again separated by the dollar symbol ("$"), but spaces and the "#" symbol are equivalent, unlike "severity 0". This is because the entire list is compared with the student response.

With "severity 7", "THE$A CAT$DOG" would would match only "THE", "A CAT" or "DOG".

(c) Input of Responses. Upon encountering a "Match" operation which requires student input (the "!MC;@" construction), the MASTER Interpreter requests input from the user. In the screen display this is characterised by the appearance of a prompt (">") and a cursor ("_"), where text was last displayed (Figure 6.1). As keys are pressed characters appear on the screen where the cursor was positioned. The inclusion of a cursor in the response entry section of the Interpreter was accompanied by a marked increase in confidence of students when answering questions, since it allowed them to edit responses more easily. In keeping with the usual editing feature of computers, the backarrow key was designed to remove characters from the response when struck.

The case of the response on the screen was designed to be a function only of a "shift-lock" key: when the ESC key

was pressed the case of the display would change. Internally however, the entire response is stored in upper case allowing the Author to match in one case only.

All of the processing implied by these requirements was designed to be performed upon the entry of each character, there being significant computer time available (as outlined in previous chapters). In this way response times to student input proved to be very satisfactory, even with complex analyses of responses.

In the teaching package the use of the "shift-lock" feature by students was rare. This was probably because it received little emphasis in any of the MASTER lessons, since the ESC key was already in use in two other programs for different purposes. By setting the default to upper case, maximum contrast between the displayed text (mostly lower case) and student input was achieved.

(c) Storing Responses. It is important to have a record of student responses, especially "during the early life" of a lesson (Nievergelt, 1980). Modification of keyword lists, question wording and even methods of teaching may result from examination of such records.

If input of a student response is requested, the Interpreter will store the entire response, providing the response is to be analysed by the Interpreter. If the "Match" is simply being used as a pause (i.e. there are no lines of keywords), the response is not stored.

If the user presses only the "Return" key in response to an "MC" operation, the phrase "NULL RESPONSE" is recorded in the response file, although the response can be matched

against the null string (in, for example, "HELP$$NO#IDEA"). The file of responses is stored onto disk when an "EXit" operation is performed.

(6) Counters

Testing of MASTER lessons revealed the need for some limited mathematical functions to be included (Chapter V). Two further operations were therefore added: "Alter Counter", to set the value of a counter and "Jump on Counter Value", to perform a simple JU depending on the value of a counter. Five counters, "%0", "%1", "%2", "%3" and "%4", were made available for use in simple arithmetic expressions.

(a) Alter Counter. Using "Alter Counter" the value of one of the counters may be defined. The format of the "AC" operation is "!AC;%c=<expression>", where "%c" is a valid counter, whose value is set to the value of the expression. The expression was designed to include small integers (from 0 to 4) and counters 1 to 4, connected by either addition or subtraction. Some examples are "%1+2", which adds 2 to counter %1 and "%3+%4", which adds counters %3 to %4.

Counter %0 was intended for use in accumulations only, with the value of the expression being added to counter %0, except when it evaluates to 0. "!AC;%0 = 1*" increments counter %0 by 1, while "!AC;%0 = 0*" sets %0 to 0.

"Alter Counter" is unique amongst operations in that it does not direct to a new node. An "AC" must therefore always be followed by another operation.

(b) Jump on counter value. The "JC" operation allows a conditional branch to be performed. It is included in a lesson in the form "!JC;%c$x;n1n2n3n4*", where "%c" is a valid counter, x the number of nodes in the list and "n1", "n2", "n3" and "n4" valid nodenames. If the value of the counter is 1, a simple "JU" is made to the first node in the list. If "2" a "jump" is made to the second and so on. Where the value of the counter is outside the range specified, a "JU" is made to the last node in the list.

The "Jump on Counter Value" has been most successfully used in conjunction with the "MC" and "AC" operations, to control the number of attempts at a question.

3. TEXT

Primarily, text associated with a node has been included for display on the screen. The appearance of the screen was left entirely to the Author of the lesson, since this appeared to be the most effective method of forcing attention to be paid to this most important aspect.

Text included in a node is displayed on the screen, commencing below the text last displayed and continuing down the screen. A "wrap-around" function was included, so that text that would have been written below the bottom of the screen appeared at the top. In addition text display was designed to be "non-destructive", adding to the current display, without erasing. Text "wrap-around" can have an undesirable appearance and is usually only useful as a development aid during Author testing.

At an early stage in the development of MASTER it was decided to simplify the basic structure of the language as far as possible. This implied that any sophisticated features, mainly for control of the screen display, had to be incorporated into the text. In keeping with the intention of simplicity the inclusion of a special feature was indicated by the "@" character, followed by one or more characters to complete the function definition.

Initially a small set of options, such as "display a benzene ring", "sound the bell" and "clear the screen", was implemented for testing by CAL Authors including, for example Temple (1986), whose project made significant use of the MASTER language. The available range was increased as a result of these investigations and the resulting options could be classed into one of three categories: direct screen display, screen formatting and program control.

(1) Screen display

Options in this category generally have an immediate effect and may be considered as representing a small number of characters.

"Display Benzene" ("@A") displays a small benzene nucleus as a part of the screen display. It has proved to be most used in the display of formulas. Propriophenone, for example, may be displayed using "@ACOCH@2CH@3".

"Display number" ("@x", where "x" is a digit) results in the display of a digit as a subscript. This function is usually used in conjunction with line spacing.

"Display counter value" ("@%c", where "%c" is a valid counter) displays the value of a counter.

"Sound Bell" ("@B") simply sounds the computer speaker, an effect commonly used to draw attention to an important feature of the display.

(2) Formatting

General control of the screen may be exercised using the eight functions in this category.

"Clear screen" ("@C") clears the entire screen, resets line spacing to 10 and causes the following text to appear at the top of the screen.

"Move to top of screen" ("@D") causes the following text to be displayed at the top of the screen.

"Erase to bottom of screen" ("@E") clears from (and including) the current line to the bottom of the screen.

"Move to bottom of the screen" ("@U") causes the following text to appear on the last line on the screen. This option causes "wrap-around" if used carelessly and is therefore used in conjunction with other moving functions. It is commonly used for prompts.

"Set position" ("@Y") stores the current vertical position, which may then be accessed by the "@M" function.

"Move to position" ("@M") causes the following text to appear at the last position set by "@Y".

"Set line spacing" ("@Ss", where "s" is a letter), sets the line spacing to a value (equivalent to the letter: A=1, B=2, ...). A spacing of less than 8 causes succeeding lines of text to overlap, making superscripts and subscripts possible.

"Display at line" ("@Ll", with "l" a letter), causes the following text to be displayed at the appropriate line

down from the top of the screen. This function depends on the current line spacing and therefore, by altering both settings, any vertical position may be specified.

(3) Program Control

The two options in this category could have been included as operations, but it was felt that this would have compromised the relative simplicity of basic lesson construction.

The first function, "Include a MASTER lesson" ("@I<lesson name>"), results in the commencement of the specified MASTER lesson. The screen display, position of next text, value of "@Y", values of counters and stored responses are retained.

"Load a compressed screen" ("@Pl<filename>") loads the specified compressed picture file stored on disk and then displays it according to the "mode" ("1"), which may be "D", "F", "J", "N" implying modes "4", "6", "10" and "14" (Apple Reference manuals).

The variety of display modes makes it possible to create a large number of displays by screen modification rather than substitution. Construction of a series of screen displays by overlaying compressed picture files has proved to be an effective method of information presentation (Chapter VI).

4. OTHER CONSIDERATIONS

When the MASTER Interpreter and several lessons were included in the teaching package, it was found that there was a significant pause between the choice of a lesson (by a single keystroke, from the initial menu) and the start of that lesson. This delay arose from the need to firstly load the Interpreter and then the actual lesson from disk into memory.

While little, apart from code optimisation, could be done about the amount of time spent loading, the pause was made less noticeable with the inclusion of a third step, between the first two. In a similar fashion to that used in other components of the teaching package, this initialisation step was somewhat disguised by the display of a compressed picture file, displaying a logo. Since the total load time rarely exceeded twenty seconds, the result proved to be very satisfactory.

Due to limitations imposed by the memory size of the computer, it occasionally proved difficult to fit all of the required material into one lesson. For this reason the capability to start a MASTER lesson from within another was included. A similar practice to that adopted when first loading the lesson therefore proved necessary when using this function. It was found that the time taken by the inclusion was apparently not noticed by students if a suitably interesting display was presented at the appropriate time.

In the teaching package two types of display were used: the first, included in the questions accompanying the

second tutorial program, consisted of a resume of the main points of an important question. The second was a "compressed" picture, loaded to introduce a new section of material in the concluding MASTER lesson. Although the latter seemed more interesting, both were effective at minimising the effect of the pause upon student concentration.

APPENDIX C

THE ACHIEVEMENT SCALE

NAME _____

Achievement Scale

The purpose of this test is to determine how effective the teaching of NMR has been in your course so far.

The results of this test will be posted on the noticeboard as soon as possible so that you may see how much work you need to do on the subject.

There are three sections in this scale, testing your knowledge of the theory, appreciation of chemical shift and ability to analyse and predict spectra of various compounds.

As this is a test of your background knowledge as well as your performance, you should include your working as far as possible, especially in the last section.

Section 1

When answering the questions in section 1, please make your intentions clear. Most of the questions have instructions on how to answer. For example :

1) Indicate whether the statement is true or false.

One metre is a longer than one yard. (TRUE) FALSE

2) Which of the following is NOT a basic SI unit?

a) The metre.
b) The gram.
c) The second.
d) All of the above are basic units.

The best answer is (a,b,c or d) ? b

3) Arrange the following into an order of decreasing length.

I metre
II chain
III furlong

The order is ?

4) The basic unit of measure is ? III II I

PLEASE TURN OVER

NMR Achievement Test

1) What are the possible values of I, the nuclear spin?

2) A nucleus with spin I, can take a number of orientations in a magnetic field.

How many orientations can the nucleus take when

I = 1 (a,b,c or d) ?

I = 5/3 (a,b,c or d) ?

a) It depends on the magnetic field
b) Less than 4
c) Greater than or equal to 4
d) None of a,b or c.

3) Give the values of the nuclear spin for the following nuclei.

^{13}C ? _____

^{1}H ? _____

^{15}N ? _____

^{12}C ? _____

^{16}O ? _____

4) In NMR resonance is achieved when the relation between the applied radiation, at frequency ν, and the field experienced at the nucleus, B, is satisfied.

The relation between ν and B is

a) linear.
b) inverse.
c) dependent on I.
d) none of the above.

Is the answer a,b,c or d ?

5) Indicate which statements are true

The gyromagnetic ratio

I	is constant.	TRUE/FALSE
II	does not depend on the magnetic field.	TRUE/FALSE
III	can be negative in certain cases.	TRUE/FALSE

PLEASE TURN OVER

6) Indicate which statements are true.

The relative chemical shift value depends on

I the magnetic field applied to the nucleus. TRUE/FALSE
II the nucleus itself. TRUE/FALSE
III the electronic environment of the nucleus. TRUE/FALSE

7) A good solvent for use in PROTON NMR would be

a) CH_3COCH_3.
b) $CDCl_3$.
c) $Si(CH_3)_4$.
d) CH_3CH_2OH.

Is the BEST answer a,b,c or d ?

8) Arrange the following types of proton into an order of decreasing chemical shift.

I $-CH=CH_2$
II $-C\equiv CH$
III $-CH_2-CH_3$

The order is ?

9) Arrange the following types of carbon into arranged into an order of decreasing chemical shift.

I CH_3-O-
II CH_3-CO-
III 

The order is ?

10) Indicate which statements are correct.

Spin-spin coupling can be observed

I in 1H NMR when there are protons on adjacent carbons. TRUE/FALSE

II when nuclei with non-zero nuclear spin are directly bonded. TRUE/FALSE

III in 13C NMR when a carbon has a proton attached. TRUE/FALSE

Section 2

This section is intended to test your appreciation of chemical shift.

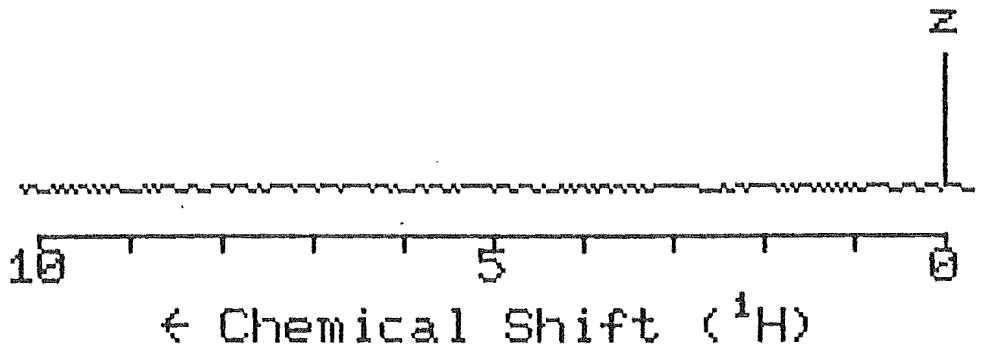
For each of the highlighted types of proton (enclosed in a box), you are required to indicate its chemical shift.

You can best do this by putting a line on the continuum provided at your estimate of the shift and labelling it with the appropriate letter.

The value for TMS (0 ppm) has been included as an example (it has the label 'z').

R is an alkyl group.

The number of protons represented by each multiplet is indicated by a number above the multiplet.



a) $\boxed{CH_3}-CH_2-R$

b) $\boxed{CH_3}-CO-R$

c) $\boxed{CH_3}-O-R$

d) $\boxed{CH_2}=CH-R$

e) 

f) $\boxed{H}-CO-R$

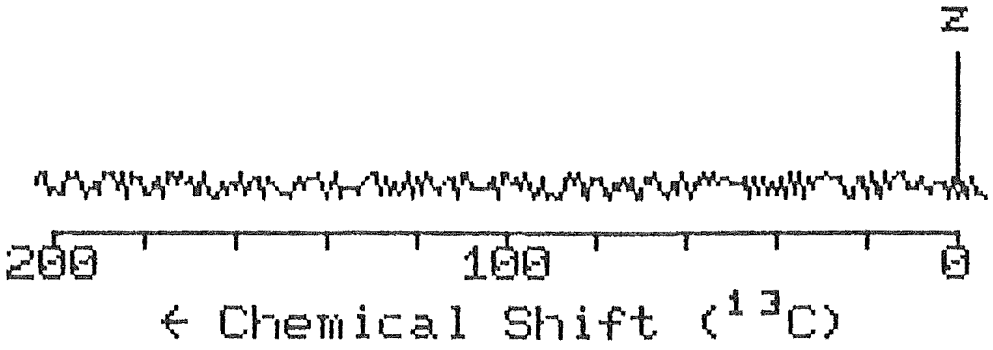
Carbon 13 Chemical Shifts

Please estimate the values of the chemical shifts for the indicated carbon groups.

Indicate each peak as a SINGLET and label it with the appropriate letter.

The example of TMS (0 ppm) is given (it has the label 'z').

R is an alkyl group.



a) $\boxed{CH_3}-CH_2-R$

b) $CH_3-\boxed{CO}-R$

c) $\boxed{CH_3}-O-R$

d) $\boxed{CH_2}=CH-R$

e) 

f) $H-\boxed{CO}-R$

Section 3

In this section your knowledge and experience with NMR spectra will be tested.

There are two types of problem in this section : the prediction of NMR spectra of compounds and the converse - the deduction of the structure of compounds.

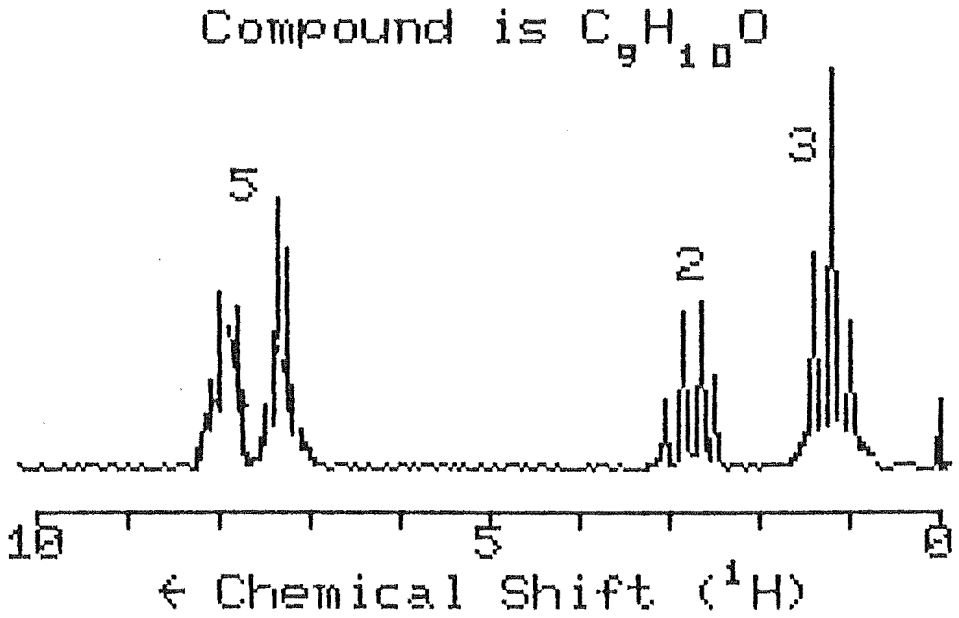
The problems become more difficult and, as credit will be given for your working, please include it.

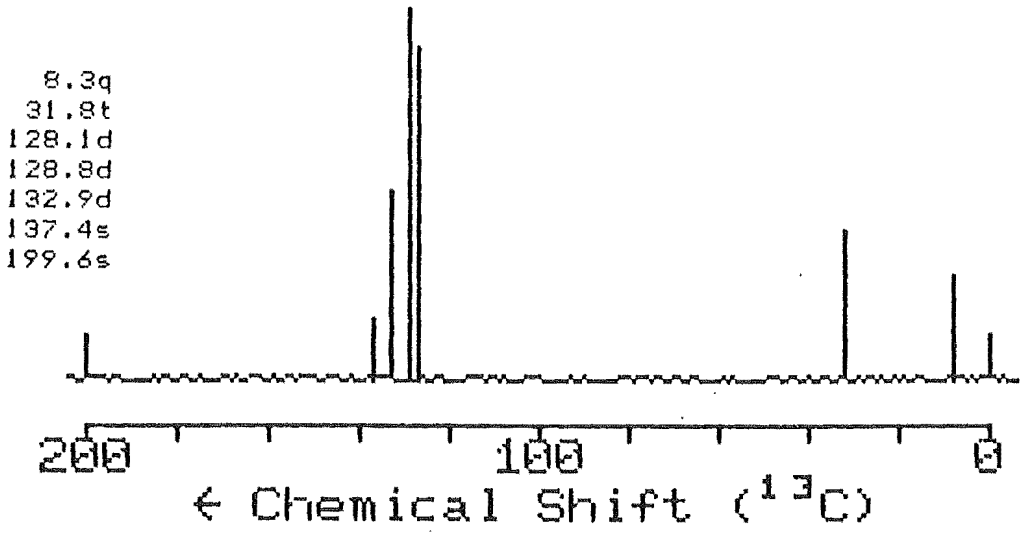
The CARBON-13 spectra are PROTON-DECOUPLED, with the splitting of each peak indicated by a letter according to the following :

s : singlet
d : doublet
t : triplet
q : quartet.

PLEASE TURN OVER

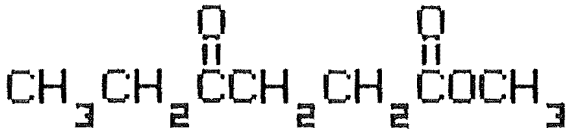
Deduce the structure of the compound from the spectra.

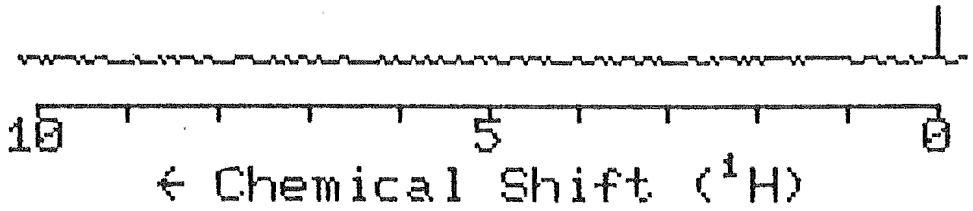




THERE IS WORKING PAPER OVER

Try to predict the PROTON NMR spectrum of

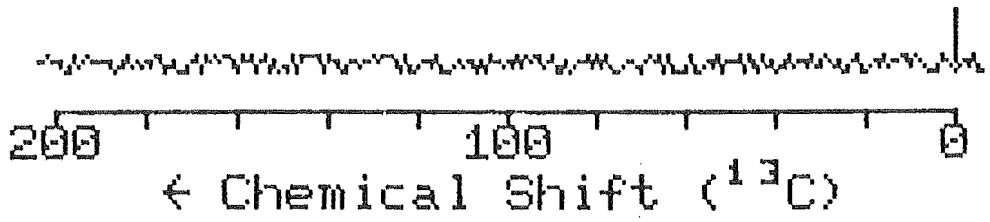




PLEASE TURN OVER

Try to predict the CARBON-13 NMR spectrum of

$$CH_3CH_2CH_2CH_2OCH{=}CH_2$$



PLEASE TURN OVER